

Mathematics Area - PhD course in
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Many-body effective equations and quantum algorithms for linear and nonlinear equations

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*La montaña nos unió pero también nos separó para siempre.
Gracias por la alegría que siempre compartiste.*

A Samu.

Abstract

Mean-field Hartree theory is a central tool for mapping interacting many-body dynamics into an effective nonlinear one-particle evolution. This approximation has been also employed when the Hamiltonian that governs the many-body dynamics is not Hermitian. Indeed, non-Hermitian Hamiltonians model particle gain/loss or the evolution of open quantum systems between consecutive quantum jumps. Furthermore, the validity of the Hartree approximation for generic non-Hermitian Hamiltonians lies at the basis of a quantum algorithm for nonlinear differential equations, where the nonlinear equation is mapped into a many-body Schrödinger equation, which may be non-Hermitian. In this application, the mean-field approximation can be seen as a linearization method, and at the end of the algorithm, the obtained linear system is solved using the Harrow-Hassidim-Lloyd (HHL) algorithm. The non-Hermitian mean-field Hartree approximation is far from being completely understood, and no rigorous results justify its applications. Instead, it is usually presented as a heuristic extension of the Hermitian case.

In the first part of this thesis, we show that this approximation can fail. We consider the most general bosonic mean-field Hamiltonian with two-body interactions and we prove that, if the Hamiltonian is not Hermitian, the Hartree equation does not capture the correct second time derivative of the one-particle marginal state at $t = 0$ in the limit of infinitely many particles. We construct a series of examples that we can solve analytically or numerically, which support the failure of the Hartree approximation and give further insight into the new phenomena that arise in non-Hermitian physics. Furthermore, we consider the mean-field evolution of open quantum systems and we show how to use the mean-field approximation of open quantum systems as a linearization method of nonlinear differential equations.

In the second part of this thesis, we study the mean-field dynamics of a Hermitian system of N interacting bosons starting from an initially condensed state. For a broad class of mean-field Hamiltonians, including models with arbitrary bounded interactions and models with unbounded interaction potentials, we prove that the probability of having n particles outside the condensate decays exponentially in n for any finite evolution time. Our results strengthen previously known bounds that provide only polynomial control on the probability of having n excitations.

Finally, we consider the HHL algorithm. Several circuit-level variants have been pro-

posed to simplify its implementation, including constructions in which the clock register is factorized via Hadamard gates to reduce circuit depth and entanglement. We provide a rigorous analysis of the convergence of the output towards the ideal solution, and we show that this commonly deployed variant can fundamentally alter the asymptotic convergence of the algorithm. This phenomenon is not a finite-size artifact and compromises the correctness guarantees of the factorized-clock implementation. We provide an analytic characterization of the underlying mechanism and propose a minimal and experimentally feasible modification that suffices to restore convergence while preserving the practical advantages of the simplified circuit. Our results clarify an overlooked correctness issue in a widely used HHL implementation pattern and delineate the conditions under which simplified realizations faithfully reproduce the intended algorithmic behavior.

List of publications

The topics presented in this thesis are based on the following publications:

- The main results of chapter 2 are based on [1] , M. Ginzburg, S. Rademacher, and G. De Palma, “Failure of the mean-field hartree approximation for a bosonic many-body system with non-hermitian hamiltonian”, arXiv preprint, `10.48550/arxiv.2601.13038` (2026)
- The main results of chapter 3 are based on [2] , M. Ginzburg, S. Rademacher, and G. De Palma, “Exponential concentration of fluctuations in mean-field boson dynamics”, arXiv preprint, `10.48550/arxiv.2602.16658` (2026)
- The main results of chapter 4 are based on [3], M. Ginzburg and U. Marzolino, “Error convergence of quantum linear system solvers”, Physical Review A **113**, 062436 (2026)

Contents

Introduction and motivations	ix
1 Overview of previous results	1
1.1 BBGKY method for Hamiltonian evolution	1
1.2 Excitation map method for Hermitian Hamiltonians	3
1.3 Non-Hermitian Hamiltonians and Lindblad evolution	6
1.3.1 Non-Hermitian Bose Hubbard dimer	6
1.3.2 Open mean-field systems	9
1.4 Quantum algorithms	11
1.4.1 Hamiltonian simulation and linear systems	11
1.4.2 Nonlinear differential equation solvers	17
2 Dissipative mean-field systems	19
2.1 The Hartree equation for non-Hermitian Hamiltonians	20
2.1.1 Short-time behavior of the reduced one-particle state	23
2.2 ZZ anti-Hermitian interaction	26
2.2.1 Large- N limit	29
2.2.2 Numerical analysis	33
2.2.3 Analysis of the second time derivative	36
2.3 Non-Hermitian ZZ interaction with real spectrum	37
2.3.1 Hermitian case	39
2.3.2 Numerical analysis of the non-Hermitian case	40
2.3.3 Analysis of the second time derivative	42
2.4 Single-particle Hamiltonian	43
2.5 Lindblad evolution	45
2.6 Conclusions and perspectives	53
3 Exponential condensation	55
3.1 Main results	56
3.2 Proof of the theorems	59
3.2.1 Excitation map revisited	59

3.2.2	Step 1	62
3.2.3	Step 2	65
3.2.4	Step 3	71
3.3	Conclusions	73
4	Quantum linear system solver	75
4.1	Error analysis	75
4.2	Improved HHL variant	79
4.3	Complexity	82
4.4	Numerical examples	83
4.5	Negative eigenvalues of A	84
4.6	Conclusions	85
A	Detailed computations	87
A.1	Steps of the HHL variant	87
A.2	Proof of Lemma 4.1.2	89
A.3	Proof of Lemma 4.1.3	93
	Bibliography	97

Introduction and motivations

Quantum many-body physics addresses the collective behavior of systems composed of a large number of interacting particles. The interactions between particles are typically dominated by pairwise forces, meaning we only need to account for how two particles interact at a time. The exact solution of many-body problems is restricted only to highly specialized integrable models and numerical simulations become intractable due to the exponential scaling of the Hilbert space with the number of particles.

Early experiments across diverse physical systems, ranging from superconductors [4] to superfluids [5] and ferromagnets [6], reveal profound quantum effects. These phenomena stem from the quantum nature of individual particles, yet they manifest primarily in the thermodynamic limit, where a macroscopic number of particles interact collectively. In this limit, the system exhibits emergent properties that cannot be deduced simply by studying a few particles in isolation. Modern experimental techniques have revolutionized this paradigm, now allowing for the precise control of individual quantum systems [7–10]. This unprecedented level of control bridges the gap between microscopic few-body interactions and macroscopic states. Nevertheless, to build a rigorous and predictive mathematical theory for complex systems, we must identify specific physical regimes where the full, high-dimensional problem simplifies.

The mean-field regime is a case where this reduction of the problem can be done. In this regime, as the number of particles becomes very large, the interaction strength is scaled down accordingly. This ensures that instead of interacting individually with every other particle, each particle moves in an effective background field created by the average density of all the other particles, allowing us to approximate the complex many-body dynamics using simpler, lower-dimensional effective equations.

A canonical example that we will have in mind is the Bose-Einstein condensation. Typical experiments on ultracold gases [11, 12], consist of trapping the particles into a potential well, and cooling them down. This system has a phase transition into a Bose-Einstein condensate, below a critical temperature there is a macroscopic concentration of the particles into a single state. As the temperature approaches zero, the particles condensate more and more into the ground state of the Hamiltonian. Once the temperature is low enough, the trap is switched off, at this point the state is not the ground state of the new Hamiltonian. If we assume that the temperature is effectively zero the particles will

evolve following the Schrödinger equation. The mean-field limit is by now well understood in a mathematically rigorous way and leads to the Hartree or Gross-Pitaevskii equations [13, 14]. Early rigorous results for the Hartree equation go back to Hepp [15]. Spohn's analysis via the BBGKY hierarchy [16] provided a general framework for bounded interactions, later extended to Coulomb potentials in [17]. Subsequent works established quantitative rates of convergence [18, 19]. A full description of the BEC would also require the study of the Gross-Pitaevskii equation. Since we will not consider this regime, we refer the reader to expand on this topic [20] for completeness.

The mathematical framework of these phenomena starts by defining the single-particle Hilbert space as the space of square-integrable functions $L^2(\mathbb{R}^3)$. A single particle is represented by a normalized wavefunction $\phi \in L^2(\mathbb{R}^3)$. The energy of a single particle consists of a kinetic contribution given by the Laplacian operator $-\Delta_x$ and a potential energy governed by an external field $V_{\text{ext}}(x)$ that defines the potential well. For the many-body system, the N -particle state $\Psi^{(N)} \in \text{Sym}^N L^2(\mathbb{R}^3)$ is a normalized wavefunction. We assume that the interaction between pairs of particles is spherically symmetric and depends only on the distance between them. At very high density, i.e., when the mean distance between particles is much smaller than the range of the interaction potential, each particle interacts with all the others in such a way that it feels a mean potential given by the average over all the pair interactions $V(x_i - x_j)$. This regime is described by the mean-field Hamiltonian

$$H_{\text{BoseGas}}^{(N)} = \sum_{i=1}^N -\Delta_{x_i} + V_{\text{ext}}(x_i) + \frac{1}{N-1} \sum_{1 \leq i < j \leq N} V(x_i - x_j). \quad (1)$$

The unitary evolution of a closed system can be described by the pure density matrix $\rho^{(N)}(t) = |\Psi^{(N)}(t)\rangle\langle\Psi^{(N)}(t)|$. Given the single-particle reduced density matrix $\rho^{(1)}(t) := \text{Tr}_{2\dots N} \rho^{(N)}(t)$, concentration of particles in a single state and the bosonic exchange symmetry implies that the single-particle reduced density matrix is approximated by a pure state $\rho^{(1)}(t) \approx |\phi(t)\rangle\langle\phi(t)|$. The Hartree equation dictates the evolution of the state ϕ after the trap is switched off,

$$i\partial_t \phi(t, x) = \left(-\Delta_x + \int dy V(x - y) |\phi(t, y)|^2 \right) \phi(t, x). \quad (2)$$

As another example, one can also be interested in considering a single-particle Hilbert space of finite dimension $\mathbb{C}^d$. Spin systems are described in this fashion with $d = 2$ and several models fit the mean-field regime [21]. One can consider that there is a lattice where the spins sit, and number each site from $1 \dots N$. Neighboring spins will interact between each other. The coordination number z is the number of neighbors for each site and it will depend on the interaction and on the lattice structure. It is a well-known result that the mean-field approximation becomes exact in the limit of $z \rightarrow \infty$ [21, 22]. In this presentation, we will restrict to systems with all to all interactions, $z = N - 1$. In this

case, the limit of infinite coordination number is the same as the thermodynamic limit. We can mention two canonical models following this structure. The fully connected Ising Hamiltonian

$$H_{Ising}^{(N)} = -\frac{J}{N} \sum_{1 \leq i < k \leq N} S_i S_k - \mathcal{B} \sum_{i=1}^N S_i. \quad (3)$$

where the S_i are Ising variables with values ± 1 , J sets the interaction strength and $\mathcal{B}$ sets the coupling to an external magnetic field. Another example is the Sherrington-Kirkpatrick model

$$H_{SK}^{(N)} = \sum_{1 \leq i < k \leq N} J_{ik} S_i S_k. \quad (4)$$

The couplings J_{ik} are random and different from zero, with a Gaussian or a bimodal distribution with variance $N^{-1/2}$ keeping the energy extensive.

All these models (1), (3), (4) have the same mean-field structure, i.e., all-to-all interactions keeping the total interaction energy extensive in the number of particles. We can summarize them in an abstract way by a generic mean-field Hamiltonian acting in the bosonic space of N particles. To be more precise, let $\text{Sym}^N \mathfrak{h}$ be the N -fold symmetric tensor product of the single-particle Hilbert space $\mathfrak{h}$. We describe the dynamics of the N bosons by a wavefunction $\Psi^{(N)}(t) \in \text{Sym}^N \mathfrak{h}$ solving the Schrödinger equation

$$i\partial_t \Psi^{(N)}(t) = H^{(N)} \Psi^{(N)}(t), \quad (5)$$

where the mean-field Hamiltonian $H^{(N)}$ is given by

$$H^{(N)} = \sum_{i=1}^N T_i + \frac{1}{N-1} \sum_{1 \leq i < j \leq N} w_{ij}. \quad (6)$$

Here, T_i denotes the self-adjoint N -particle operator acting as the self-adjoint single-particle operator $T : \mathfrak{h} \rightarrow \mathfrak{h}$ on the i -th particle and as the identity on all the other particles. Similarly, w_{ij} denotes the self-adjoint two-body interaction acting as the self-adjoint operator $w : \mathfrak{h}^{\otimes 2} \rightarrow \mathfrak{h}^{\otimes 2}$ on the particles i and j and as the identity on all the remaining particles. If T or w are unbounded, their domain is a dense subspace of $\mathfrak{h}$ or $\mathfrak{h}^{\otimes 2}$ rather than the full $\mathfrak{h}$ or $\mathfrak{h}^{\otimes 2}$, respectively. In accordance with bosonic symmetry, we assume that w is invariant under permutation of the two particles.

Motivated by the experimental realization of Bose gases, we study the many-body dynamics (5) for initial data given by a condensate state

$$\Psi^{(N)}(0) = \sum_{n=0}^N \phi(0)^{\otimes (N-n)} \otimes_s \xi^{(n)}, \quad (7)$$

where $\phi(0) \in \mathfrak{h}$ is the initial condensate wavefunction, $\xi^{(n)} \in \text{Sym}^n \mathfrak{h}$ are the n -particle wavefunctions describing the excitations orthogonal to the condensate state, and $\otimes_s$ is the

symmetrized tensor product. One can also consider the simplest case $\xi^{(n)} = 0 \forall n > 0$ given by a product state initial condition $\Psi^{(N)}(0) = \phi(0)^{\otimes N}$.

The mean-field approximation proposes that $\rho^{(1)}(t) \approx |\phi(t)\rangle\langle\phi(t)|$ in a sense that will be made rigorous later. The condensate wavefunction $\phi(t) \in \mathfrak{h}$, satisfying $\|\phi(t)\|_2 = 1$, is expected to evolve according to the Hartree equation

$$i\partial_t\phi(t) = H_H^{\phi(t)}\phi(t), \quad H_H^{\phi(t)} = T + w^{\phi(t)}, \quad (8)$$

where the effective one-particle operator $w^{\phi(t)}$ is defined through

$$\langle\varphi_1, w^{\phi(t)}\varphi_2\rangle = \langle\varphi_1 \otimes \phi(t), w \varphi_2 \otimes \phi(t)\rangle, \quad \forall \varphi_1, \varphi_2 \in \mathfrak{h}. \quad (9)$$

If w is bounded, the Hartree equation (8) always has a unique mild solution defined for any $t \in \mathbb{R}$ from [23, Chapter 6, Theorem 1.4]. For the Bose gas Hamiltonian (1), the existence and uniqueness of a mild solution of the Hartree equation (2) is also guaranteed for the coulomb potential [18]. In section 1.2 we will show that the approximation $\rho^{(1)}(t) \approx |\phi(t)\rangle\langle\phi(t)|$ can be related to a low probability of finding particles in the evolved state $\Psi^{(N)}(t)$ that are orthogonal (excited) with respect to the condensate state $\phi(t)$. There are several bounds in the literature for the concentration of the many-body wavefunction into the Hartree solution [24–32], which show that the probability of finding n particles in an excited state decreases as an inverse polynomial in n .

Historically, this approximation was introduced to simplify computations in order to have predictive theories. Since it is not possible to solve the Schrödinger equation for a macroscopic number of particles, the reduction to the single-particle Hartree equation allows to solve a simpler problem that approximates the full equation by paying the price of having a nonlinear equation.

This approximation can be used in the other direction to solve general partial differential equations. Lloyd et.al. [33] proposed a quantum algorithm where the approximation is used as a linearization method where a nonlinear partial differential equation is approximated by a linear equation for a system composed of many copies of the original system. In this case, we pay the price of having many degrees of freedom, but quantum computers are very efficient at solving linear systems, thus leading to a more efficient algorithm. Since every numerical digital computation requires some discretizations, we now restrict ourselves to the case of a finite-dimensional Hilbert space $\mathfrak{h} = \mathbb{C}^d$.

Assume that we want to solve a nonlinear differential equation that happens to match the form of the Hartree equation (8). Even if it is a single-particle equation, when the dimension becomes larger, the simulation on a classical computer becomes harder, and for systems of large dimensions it becomes infeasible to simulate. The equation solver proposes to construct a Schrödinger linear equation like (5) that approximates the original partial differential equation and can be then simulated by a quantum computer. Since the nonlinear partial differential equation is generic, the corresponding Schrödinger linear equation may or may not describe a quantum system. If it does, it can be solved using quantum

simulators [34–36] which allow one to simulate the dynamics of quantum systems governed by the Schrödinger equation. If the corresponding Schrödinger linear equation does not describe a quantum system one can use the HHL algorithm [37], which solves algebraic linear systems of equations. In both cases, the running time of the best-known classical linear solver algorithms scales exponentially with the dimension d , while the quantum algorithms scale linearly in d .

In order to compare quantum and classical algorithms, we should consider the dimension d , which makes it harder for the classical computer to solve the problem, and the number of copies N required by this linearization method to make the error small. For d large enough, this trade-off makes quantum computers more efficient than classical ones. They also proposed that the same algorithm can be applied to solve general nonlinear equations assuming that the mean-field approximation holds for non-Hermitian operators, but this assumption is not justified.

Non-Hermitian mean-field models also arise effectively in atomic, optical, condensed-matter, and photonic platforms [38–44], where they describe mechanisms of particle gain and loss. Particle losses in many-body systems are often modeled by Markovian master equations of Gorini-Kossakowski-Lindblad-Sudarshan form [45, 46]. Conditioning such dynamics on the absence of quantum jumps leads to an effective non-unitary evolution generated by a non-Hermitian Hamiltonian; this quantum-trajectory viewpoint underlies standard methods in quantum optics and atomic, molecular and optical many-body physics [47–51]. Furthermore, in cold-atom settings, controlled dissipation and losses are not merely imperfections but resources, enabling the preparation of correlated states [52, 53]. Mean-field approximations for non-Hermitian systems are used in the physics literature applied to dissipative Bose-Hubbard dimers [54–56], pumped waveguide transport [57], and tunneling in trapped systems [58], but no rigorous justification is known yet. Related progress exists for open quantum systems governed by Lindblad dynamics in the thermodynamic limit with clustering states [59–62]. However, these results do not directly address the validity of mean-field approximations for general non-Hermitian Hamiltonians, for which no systematic theoretical understanding is available.

In this thesis, we address three different subjects related to the mean-field Hartree theory and quantum algorithms. We start in chapter 1 with a general overview of these topics and previous results. In chapter 2 we discuss the generalization of the mean-field theory to non-Hermitian Hamiltonians and open quantum systems, and we show that the approximation may fail when the Hamiltonian is non-Hermitian. In chapter 3 we discuss rigorous bounds on the concentration of the many-body wavefunction into the Hartree state and we prove new, stronger bounds. Finally, in chapter 4 we analyze the HHL algorithm, used as a subroutine in the quantum nonlinear solver, and we propose a modification to it, improving the performance for some range of parameters.

Chapter 1

Overview of previous results

This chapter is dedicated to putting the whole work into context and to review the main results of the literature that will be used. In section 1.1 and section 1.2, we review the BBGKY hierarchy and the excitation map, respectively. These are two different approaches used to prove that the Hartree approximation describes exactly the dynamics of the one-particle reduced density matrix of the many-body system in the mean-field regime in the thermodynamic limit. In section 1.3, we show how the Hartree approximation is used in the literature in the context of non-Hermitian and open quantum systems. Lastly, in section 1.4, we review the most relevant quantum algorithms for solving linear and nonlinear equations.

1.1 BBGKY method for Hamiltonian evolution

Let us start by describing the BBGKY method used in [16]. The goal is to make rigorous and prove the approximation $\rho^{(1)}(t) \approx |\phi(t)\rangle\langle\phi(t)|$. This approach shifts the focus from the full N -body wave function $\Psi^{(N)}(t)$ to the sequence of reduced density matrices (or marginals) $\rho^{(k)}(t)$, defined by

$$\rho^{(k)}(t) := \text{Tr}_{k+1, \dots, N} \left(|\Psi^{(N)}(t)\rangle\langle\Psi^{(N)}(t)| \right). \quad (1.1)$$

We avoid explicitly writing the N dependence of $\rho^{(k)}(t)$ to simplify the notation, but it is worth keeping in mind this dependence. The main result is the trace convergence of the single-particle reduced density matrix to the Hartree solution

$$\lim_{N \rightarrow \infty} \text{Tr} \left| \rho^{(1)}(t) - |\phi(t)\rangle\langle\phi(t)| \right| = 0. \quad (1.2)$$

The Schrödinger evolution (5), implies that the time evolution of the full density matrix $\rho^{(N)}(t)$ is governed by the Liouville-von Neumann equation

$$i\partial_t \rho^{(N)}(t) = [H^{(N)}, \rho^{(N)}(t)]. \quad (1.3)$$

By applying the partial trace $\text{Tr}_{k+1\dots N}$, with $k = 1 \dots N - 1$ to this equation, one obtains a coupled system of equations, where the evolution of the k -th marginal depends on the $(k + 1)$ -th marginal due to the pairwise interaction w . This system of coupled equations is called the BBGKY hierarchy and it has the following form,

$$\begin{aligned} i\partial_t \rho^{(k)}(t) &= \sum_{j=1}^k [T_j, \rho^{(k)}(t)] + \frac{1}{N-1} \sum_{1 \leq i < j \leq k} [w_{ij}, \rho^{(k)}(t)] \\ &+ \frac{N-k}{N-1} \sum_{j=1}^k \text{Tr}_{k+1} [w_{j,k+1}, \rho^{(k+1)}(t)]. \end{aligned} \quad (1.4)$$

In the thermodynamic limit ($N \rightarrow \infty$), and for each fixed k , the second term on the right-hand side (internal interactions among the k particles) vanishes as $\mathcal{O}(k^2/N)$. Formally, the hierarchy "collapses" into the infinite Hartree hierarchy:

$$i\partial_t \rho_\infty^{(k)}(t) = \sum_{j=1}^k [T_j, \rho_\infty^{(k)}(t)] + \sum_{j=1}^k \text{Tr}_{k+1} [w_{j,k+1}, \rho_\infty^{(k+1)}(t)]. \quad (1.5)$$

The critical observation made by Spohn is that this infinite hierarchy admits a factorized solution of the form $\rho_\infty^{(k)}(t) = |\phi(t)\rangle\langle\phi(t)|^{\otimes k}$, provided the initial state is similarly factorized. In this case, the first equation of the hierarchy ($k = 1$) decouples and reduces exactly to the nonlinear Hartree equation (8).

The mathematical challenge, addressed by Spohn and subsequently refined for singular potentials by Erdős and Yau [17], lies in proving the uniqueness of the solution to the infinite hierarchy in an appropriate trace-class topology, thereby justifying the convergence $\rho^{(k)}(t) \xrightarrow[N \rightarrow \infty]{w^*} |\phi(t)\rangle\langle\phi(t)|^{\otimes k}$ for all $k \geq 1$. Since the limit is a rank-one projection, weak convergence immediately implies convergence in trace norm.

The construction of the BBGKY hierarchy and its extension to non-Hermitian Hamiltonians will be a central ingredient in the analysis of section 2.1. In particular we will show that new terms related to the anti-Hermitian part of the Hamiltonian arise in such an extension preventing one from taking the formal limit, $N \rightarrow \infty$, as it was done in (1.5).

The BBGKY method is based on a topological argument, therefore, it can not give a quantitative rate of convergence. The following works address this problem by using functional analysis methods. There are two main approaches in this direction, depending on whether one considers the initial state to be a coherent state in the Fock space with expected number of particles equal to N or an exact N -particle state. We will work with states of a fixed number of particles since this is the relevant case for application in quantum algorithms.

1.2 Excitation map method for Hermitian Hamiltonians

In this section we review the excitation map, introduced in [63] to study the ground state of mean-field Hamiltonians of Bose gases (1), assuming the operator inequality $V^2 \leq D(1-\Delta)$ for some constant $D > 0$. In [25] they applied the excitation map to study the dynamics of this system and we adapt some of their definitions to the notation that will be used in chapter 3.

The excitation map is based on the idea that while the one-particle Hilbert space $\mathfrak{h}$ has a decomposition into $\mathfrak{h} = \text{span}(\{\phi(t)\}) \oplus \text{span}(\{\phi(t)\})^\perp$, the N -particle Hilbert space $\text{Sym}^N \mathfrak{h}$ has a decomposition into products of $\text{span}(\{\phi(t)\})$ and

$$\mathcal{F}_{\perp \phi(t)}^{\leq N} := \bigoplus_{n=0}^N \text{Sym}^n \mathfrak{h}_+(t), \quad (1.6)$$

with $\mathfrak{h}_+(t) = \text{span}(\{\phi(t)\})^\perp$ called the orthogonal or excitation Fock space. More precisely, any state $\psi^{(N)} \in \text{Sym}^N \mathfrak{h}$ can be written using the decomposition into the Hartree state at a fixed time and its orthogonal complement as

$$\psi^{(N)} = \sum_{n=0}^N \phi(t)^{\otimes (N-n)} \otimes_s \zeta^{(n)}, \quad (1.7)$$

for some appropriate, uniquely defined, $\zeta^{(n)} \in \text{Sym}^n \mathfrak{h}_+$.

In contrast to the standard bosonic Fock space

$$\mathcal{F} := \bigoplus_{n=0}^{\infty} \text{Sym}^n \mathfrak{h}, \quad (1.8)$$

the orthogonal Fock space is defined over $\mathfrak{h}_+(t)$ (instead of $\mathfrak{h}$) and contains wavefunctions of at most N particles. On the Fock space $\mathcal{F}$, we have the usual creation and annihilation operators given by

$$a_i^* = a^*(e_i), \quad \text{and} \quad a_i = a(e_i), \quad (1.9)$$

where we set $e_0 := \phi(t)$ and $\{e_i\}_{i \in \mathbb{N}_+}$ as an orthonormal basis of $\text{span}(\{\phi(t)\})^\perp$. These operators also define the number of particles operator

$$\mathcal{N} = \sum_i a_i^* a_i. \quad (1.10)$$

We note that to simplify the notation, we neglect the time dependence of the basis $\{e_i\}_{i \in \mathbb{N}_+}$ and e_0 in their notation. It is important to keep in mind that the operators a_i^*, a_i are time

dependent, but since $\mathcal{N}$ is independent of the basis, it is also independent from time. The creation and annihilation operators satisfy the standard canonical commutation relations

$$[a_i^*, a_j^*] = [a_i, a_j] = 0, \quad \text{and} \quad [a_i, a_j^*] = \delta_{ij}. \quad (1.11)$$

The excitation map is a time-dependent operator defined in order to act over N -particle states by destroying all the particles in the condensate and returns a state in the orthogonal Fock space. It is defined as $U_{N,t} : \text{Sym}^N \mathfrak{h} \rightarrow \mathcal{F}$ and acts as follows

$$U_{N,t} \sum_{n=0}^N \phi(t)^{\otimes(N-n)} \otimes_s \zeta^{(n)} = \bigoplus_{n=0}^N \zeta^{(n)}. \quad (1.12)$$

By definition, the image is the orthogonal Fock space. One can check that its adjoint operator $U_{N,t}^* : \mathcal{F} \rightarrow \text{Sym}^N \mathfrak{h}$, is defined by

$$U_{N,t}^* \bigoplus_{n=0}^{\infty} \zeta^{(n)} = \sum_{n=0}^N \phi(t)^{\otimes N-n} \otimes_s \zeta^{(n)}, \quad (1.13)$$

and it is a partial isometry, since $U_{N,t}^* U_{N,t}$ is the identity operator and $U_{N,t} U_{N,t}^*$ is a projector over $\mathcal{F}_{\perp \phi(t)}^{\leq N}$.

The main object studied in [25] is the excitations vector defined as

$$\Xi_{N,t} := U_{N,t} \Psi^{(N)}(t), \quad (1.14)$$

where $\Psi^{(N)}(t)$ is the solution of the N -particle mean-field Schrödinger equation, with Hamiltonian (1), and $V_{ext} = 0$. $U_{N,t}$ is defined as in (1.12) with $\phi(t)$ the solution of the Hartree equation (2).

They showed that, in the limit $N \rightarrow \infty$, the excitations vector converges to the state $\Xi_t = \bigoplus_{n=0}^N \xi^{(n)}(t) \in \mathcal{F}_{\perp \phi(t)}^{\leq N}$ satisfying the Bogoliubov equation

$$i\partial_t \Xi_t = \mathbb{H} \Xi_t, \quad (1.15)$$

for some explicit quadratic Bogoliubov Hamiltonian $\mathbb{H}$. Observe that N -particle product states are mapped to the vacuum by the excitation map, $U_{N,t} \phi^{\otimes N} = \Omega$. They showed that even if the initial state is a product state, and then $\Xi_0 = \Omega$, the Bogoliubov evolution (1.15) gives a non trivial excitations vector for any finite time. And this shows that $\Psi^{(N)}(t)$ does not stay close in norm to a pure product state.

The main result expresses this idea by studying the convergence at the level of the N -particle wave function. They showed the convergence $\Xi_{N,t} \rightarrow \Xi_t$ strongly in $\mathcal{F}$, which can be translated to

$$\lim_{N \rightarrow \infty} \left\| \Psi^{(N)}(t) - \sum_{n=0}^N \phi(t)^{\otimes(N-n)} \otimes_s \xi^{(n)}(t) \right\| = 0. \quad (1.16)$$

This result is stronger than the convergence of the reduced density matrices (1.2). Indeed, if we restrict to the computation of the k -particle reduced density matrix for fixed k , each term $\phi(t)^{\otimes(N-n)} \otimes_s \xi^{(n)}(t)$ has a finite number of excitations and then at first order in the limit $N \rightarrow \infty$, the only contribution comes from the Hartree state and then one has as a corollary that

$$\lim_{N \rightarrow \infty} \text{Tr} \left| \rho^{(k)}(t) - |\phi(t)\rangle\langle\phi(t)|^{\otimes k} \right| = 0 \quad (1.17)$$

for every fixed $k > 0$.

Furthermore, one can quantify the convergence for finite N by counting the number of particles in a state orthogonal to the Hartree state. In Lemma 14 from [25] they used Gronwall's lemma and the excitation map formalism to prove the bound

$$\langle \Xi_{N,t}, (\mathcal{N} + 1) \Xi_{N,t} \rangle \leq C e^{Ct} \langle \Xi_{N,0}, (\mathcal{N} + 1) \Xi_{N,0} \rangle. \quad (1.18)$$

We will use this type of bounds, so it is useful to make some comments about the relation between the number of excitations and the convergence of the reduced density matrix. Particles outside the condensate are counted by the excitation number operator

$$\mathcal{N}_+(t) = \sum_{i=1}^N Q(t)_i, \quad (1.19)$$

where $Q(t)_i$ denotes the operator acting as the orthogonal projector $Q(t) = 1 - |\phi(t)\rangle\langle\phi(t)|$ on the i -th particle and as the identity on all others. With this notation, condensation at positive times can be expressed by

$$\frac{1}{N} \langle \Psi^{(N)}(t), \mathcal{N}_+(t) \Psi^{(N)}(t) \rangle \rightarrow 0 \quad \text{as } N \rightarrow \infty. \quad (1.20)$$

Using the particle exchange symmetry one can relate (1.20) to the infidelity between the single-particle reduced density matrix and the Hartree solution,

$$I := 1 - \langle \phi(t), \rho^{(1)}(t) \phi(t) \rangle = \frac{1}{N} \langle \Psi^{(N)}(t), \mathcal{N}_+(t) \Psi^{(N)}(t) \rangle. \quad (1.21)$$

Convergence in number of particles (1.20) and in trace norm (1.2) are equivalent in the sense that one implies the other, but their rates of convergence are not the same, see, e.g. [13].

Using the excitation map, we will show later that $\mathcal{N}_+(t) = U_{N,t}^* \mathcal{N} U_{N,t}$. Then the result (1.18) implies (1.20) with a rate of convergence $\mathcal{O}(e^{Ct}/N)$.

More recently, these results have been refined by proving uniform bounds on higher moments of the excitation number,

$$\langle \Psi^{(N)}(t), (\mathcal{N}_+(t))^k \Psi^{(N)}(t) \rangle = \mathcal{O}(1), \quad (1.22)$$

for fixed $k \in \mathbb{N}$ in the limit $N \rightarrow \infty$; see, for example, [24–32].

We will dedicate chapter 3 to the proof of new stronger bounds on the number of excitation using the techniques described in this section.

1.3 Non-Hermitian Hamiltonians and Lindblad evolution

The Schrödinger equation (5) describes a unitary evolution, in order to introduce dissipative processes within the system, there are two different approaches, leading to non-unitary evolutions. The phenomenological approach adds non-Hermitian terms into the Hamiltonian, this modification leads to new phenomena that are not present in the Hermitian case, a comprehensive review can be found here [43] and a recent discussion of applications into many-body systems is given in [44]. The mean-field regime of non-Hermitian Hamiltonians is not yet understood, in [55] they analyze the classical limit of non-Hermitian quantum dynamics and in [56] they applied it to the dissipative Bose-Hubbard dimer and we will review it in subsection 1.3.1. This approach has also been used in [57, 58].

A more fundamental approach to introduce dissipative processes into quantum system is given by the theory of open quantum systems. A comprehensive review of the whole subject can be found here [64]. This approach has been applied to mean-field systems, it describes effects like the super-radiance studied by [65, 66], the fully connected dissipative XYZ model studied in [67], and the Zeno effect described in [51] and experimentally demonstrated in [53]. Mathematical studies of the mean-field regime of open quantum systems go back to [68], and we will review it in subsection 1.3.2. The proof follows the BBGKY approach, then it does not provide any bound on the rate of convergence. A different approach is given by [59]. They give bounds on the convergence towards the effective equation. But we will not use this result because they consider a different Lindbladian.

1.3.1 Non-Hermitian Bose Hubbard dimer

As a typical example of how the mean-field approximation is used for non-Hermitian Hamiltonians in the literature, we will now review the approach used in [56]. They considered a two-dimensional single-particle Hilbert space, and the operators $a_i^\dagger$, that create bosonic particles in modes $i = 1, 2$. They introduced the following N -particle Hamiltonian in the second quantization,

$$H_{\text{dimer}} = \varepsilon \left(a_1^\dagger a_1 - a_2^\dagger a_2 \right) - 2i\gamma a_1^\dagger a_1 + \nu \left(a_1^\dagger a_2 + a_1 a_2^\dagger \right) + \frac{c}{2} \left(a_1^\dagger a_1 - a_2^\dagger a_2 \right)^2. \quad (1.23)$$

The dissipation term describes the decay of particles in mode 1. Even if the total number of particles $\mathcal{N} := a_1^\dagger a_1 + a_2^\dagger a_2$ commutes with the Hamiltonian, its expectation value is not a conserved quantity, and the losses of particles in mode 1 increase the relative probability of finding particles at the state 2. The interaction strength c scales with the number of particles in such a way that, in the thermodynamic limit $N \rightarrow \infty$, the product $Nc = g$ is fixed. This way we recover the typical scaling of the mean-field Hamiltonian (6).

The Hamiltonian can be expressed in the form of an angular momentum system, fol-

lowing the Schwinger representation

$$L_x = \frac{1}{2} \left(a_1^\dagger a_2 + a_1 a_2^\dagger \right), \quad L_y = \frac{1}{2i} \left(a_1^\dagger a_2 - a_1 a_2^\dagger \right), \quad L_z = \frac{1}{2} \left(a_1^\dagger a_1 - a_2^\dagger a_2 \right). \quad (1.24)$$

They obey the usual SU(2) commutation relation

$$[L_x, L_y] = iL_z, \quad (1.25)$$

and its cyclic permutations. The Hamiltonian (1.23) can be reformulated in the form

$$H_{\text{dimer}} = 2(\epsilon - i\gamma)L_z + 2vL_x + 2cL_z^2 - i\gamma\mathcal{N}. \quad (1.26)$$

Using the Schrödinger equation $i\partial_t\Psi = H_{\text{dimer}}\Psi$, and given the Hermitian and anti-Hermitian part of the Hamiltonian $H_{\text{dimer}} = \mathcal{R} - i\Gamma$, where both $\mathcal{R}, \Gamma$ are Hermitian operators, the norm of Ψ is not conserved and it satisfies

$$\partial_t \langle \Psi, \Psi \rangle = -2\langle \Psi, \Gamma \Psi \rangle. \quad (1.27)$$

Let us define normalized expectation values of operators as $\langle \cdot \rangle = \frac{\langle \Psi, (\cdot) \Psi \rangle}{\langle \Psi, \Psi \rangle}$. Then for any time independent operator O , it satisfies the equation

$$i\partial_t \langle O \rangle = \langle [O, \mathcal{R}] \rangle - i \left(\frac{1}{2} \langle \{O, \Gamma\} \rangle - \langle O \rangle \langle \Gamma \rangle \right). \quad (1.28)$$

They propose the following heuristic approach, motivated by the Hermitian case. The mean-field approximation is equivalent to the assumption that the many-particle state, initially chosen as a product state

$$|x\rangle = \frac{1}{\sqrt{N!}} \left(x_1 a_1^\dagger + x_2 a_2^\dagger \right)^N |0, 0\rangle, \quad (1.29)$$

remains approximately a product state for all times of interest. This assumption is in fact exact for vanishing interaction $c = 0$. Under this assumption, every expectation value can be written as product of the expectation values $\langle L_i \rangle$ for $i = x, y, z$. In particular, we have

$$\begin{aligned} \langle \{L_i, L_j\} \rangle &= 2 \left(1 - \frac{1}{N} \right) \langle L_i \rangle \langle L_j \rangle + \delta_{ij} \frac{N}{2}, \\ \langle \{L_i, N\} \rangle &= 2N \langle L_i \rangle. \end{aligned} \quad (1.30)$$

This allows us to define the classical variables $s_i = \langle L_i \rangle / N$ and then the equation (1.28) is written as the Hartree equation

$$\begin{aligned} \partial_t s_x &= -2\epsilon s_y - 4g s_y s_z + 4\gamma s_x s_z, \\ \partial_t s_y &= +2\epsilon s_x + 4g s_x s_z - 2v s_z + 4\gamma s_y s_z, \\ \partial_t s_z &= 2v s_y - \gamma (1 - 4s_z^2). \end{aligned} \quad (1.31)$$

In [56] they compare the evolution of s_i given by the Hartree equation (1.31) with the numerical simulation of the evolution of $\langle L_i \rangle / N$ using the exact N -body Schrödinger equation. They observed that the qualitative behavior is similar for different values of the parameters in the Hamiltonian (1.23). However, since numerical simulations allow one to consider up to $N = 30$, this approach is not enough to conclude on the thermodynamic limit or to have quantitative results.

Now we rewrite some of the equations in order to make the comparison easier between [56] and the presentation of chapter 2. The Hamiltonian (1.23) can be compared with the mean-field operator (2.1) if we write it in first quantization. Each particle has two possible modes, then the internal Hilbert space has dimension two and we can define the Pauli operators X_i, Y_i, Z_i acting on the i -th particle. The restriction of the angular momentum operators to the Fock sector of fixed number of particles is given by the following relations

$$\begin{cases} L_x|_{\mathcal{N}=N} = \frac{1}{2} \sum_{i=1}^N X_i \\ L_y|_{\mathcal{N}=N} = \frac{1}{2} \sum_{i=1}^N Y_i \\ L_z|_{\mathcal{N}=N} = \frac{1}{2} \sum_{i=1}^N Z_i \end{cases} \quad (1.32)$$

The action of (1.23) restricted to N -particles is

$$H_{\text{dimer}}^{(N)} = \sum_{i=1}^N (-2i\gamma \mathbb{I} + (\varepsilon - 2i\gamma)Z + \nu X)_i + \frac{1}{N} \sum_{1 \leq i < j \leq N} g Z_i Z_j. \quad (1.33)$$

Changing the factor $1/N$ by $1/(N-1)$ creates a correction $\mathcal{O}(1/N^2)$, which does not affect any calculation.

Let us show that the evolution equation for the expectation values of operators (1.28) is equivalent to the non-Hermitian von Neumann equation (2.3) for the normalized density matrix. Let us define $\hat{\rho}^{(N)} = |\Psi\rangle\langle\Psi|/\langle\Psi|\Psi\rangle$. Then (1.28) is written as

$$\text{Tr} \left(O i \partial_t \hat{\rho}^{(N)} \right) = \text{Tr} \left(O \left([\mathcal{R}, \hat{\rho}^{(N)}] - i \{ \Gamma, \hat{\rho}^{(N)} \} + 2i \text{Tr} \left(\Gamma \hat{\rho}^{(N)} \right) \hat{\rho}^{(N)} \right) \right). \quad (1.34)$$

Since this equation holds for any observable O , it implies that

$$i \partial_t \hat{\rho}^{(N)} = H_{\text{dimer}}^{(N)} \hat{\rho}^{(N)} - \hat{\rho}^{(N)} \mathcal{H}^{(N)\dagger} - \text{Tr} \left(\left(H_{\text{dimer}}^{(N)} - H_{\text{dimer}}^{(N)\dagger} \right) \hat{\rho}^{(N)} \right). \quad (1.35)$$

This is equivalent to the non-Hermitian von Neumann equation (2.3). And a similar computation shows that the Hartree equation (1.31) is equivalent to the Hartree equation for the single-particle reduced density matrix $\hat{\rho}^{(1)}$ given in (2.9). The key observation is that the three momentum operators L_i , when they are restricted to the Fock sector of a single particle, they form a base of single-particle observable operators $\{X, Y, Z\}$ and then all the information in s_i is enough to reconstruct $\hat{\rho}^{(1)}$.

The key assumption (which is not justified) is that the state is a product at all times and it implies equation (1.30). This allows one to write the expectation values of two-particle

operators, related to $\hat{\rho}^{(2)}$, in terms of the expectation value of single-particle operators, related to $\hat{\rho}^{(1)}$. In the context of the BBGKY hierarchy approach, this relation between $\rho^{(2)}$ and $\rho^{(1)}$ is the one that allows one to close the hierarchy and write an effective evolution in terms of the single particle.

1.3.2 Open mean-field systems

The fundamental approach to open quantum systems associates the dissipative processes of the system to the interaction with an environment, in such a way that the full system evolves unitarily. Let $\mathcal{H}_S$ and $\mathcal{H}_B$ be the Hilbert spaces of the system and of the environment, and consider $S(\mathcal{H}_S)$ as the space of density matrices. If they are isolated from one another, each system evolves unitarily with the corresponding Hamiltonians H_S and H_B . The interaction between them is given by the Hamiltonian H_I . Given a fixed time $t > 0$, the operator $U(t) = e^{-i(H_S+H_B+H_I)t}$ describes the unitary evolution of the full system. Assume the initial state of the full system is given by the uncorrelated product state $\rho_{full}(0) = \rho(0) \otimes \rho_B$, then, it will evolve to $\rho_{full}(t) = U(t)\rho_{full}(0)U(t)^\dagger$. Since we are interested in the evolution of the system, we use the notion of partial trace to define $\rho(t) := \text{Tr}_B(\rho_{full}(t))$. The evolution of the density matrix of the system follows a non unitary evolution given by the dynamical map $V(t)$, which is defined by the following commutative diagram,

$$\begin{array}{ccc} \rho_{full}(0) = \rho(0) \otimes \rho_B & \xrightarrow{\text{unitary evolution}} & \rho_{full}(t) = U(t,0) \rho(0)_{full} U^\dagger(t,0) \\ \text{Tr}_B \downarrow & & \text{Tr}_B \downarrow \\ \rho(0) & \xrightarrow{\text{dynamical map}} & \rho(t) = V(t)\rho(0) \end{array}$$

or equivalently

$$\rho(t) = V(t)\rho(0) = \text{Tr}_B(U(t,0) \rho(0) \otimes \rho_B U^\dagger(t,0)). \quad (1.36)$$

The definition of the dynamical map involves operators on the full Hilbert space, but since it is a map from $S(\mathcal{H}_S)$ into itself, it can be characterized completely in terms of operators pertaining to the open system's Hilbert space $\mathcal{H}_S$.

Under the assumption that the characteristic time scales over which the reservoir correlation functions decay are much smaller than the characteristic time scale of the system's evolution, it is justified to neglect memory effects in the reduced system dynamics. As in the classical theory one thus expects Markovian-type behavior,

$$V(t_1 + t_2) = V(t_1)V(t_2) \quad \forall t_1, t_2 \geq 0. \quad (1.37)$$

The family of dynamical maps for $t \geq 0$ satisfying (1.37) is called a quantum dynamical semi-group. Mathematically, it forms a completely positive semi-group, and they were initially studied by [45, 46]. In these foundational papers, they proved that it can be

written in the form $V(t) = e^{\mathcal{L}t}$ where the generator $\mathcal{L}$ is called the Lindbladian. And the most general form of the generator is given by

$$\mathcal{L}\rho = -i[H, \rho] + \sum_k \left(L_k \rho L_k^\dagger - \frac{1}{2} \{L_k^\dagger L_k, \rho\} \right) \quad \forall \rho \in S(\mathcal{H}_S), \quad (1.38)$$

where the operators L_k are the Lindblad jump operators representing the specific dissipative channels induced by the environment and H is the coherent effective system Hamiltonian, which includes both the dynamics of H_S and also the remaining terms induced from the environment. See [64] for a detailed microscopic derivation of these operators from the full system Hamiltonian. One arrives then to the celebrated Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) master equation

$$\partial_t \rho(t) = \mathcal{L}\rho(t). \quad (1.39)$$

Following [64], there are two different scenarios where one can consider a mean-field regime for open quantum systems.

In the first scenario, one considers a mean-field system that is coupled to an external bath. From the mean-field Hamiltonian, it is possible to derive the single-particle nonlinear Hartree equation. One can approximate the coupling of the environment by a coupling to this effective single particle and arrive at the effective single-particle master equation which is linear in the dissipative term. There is no rigorous analysis of this approximation, and we will not give any more details on this approach. An application of this method is given in [64, 3.7.3 mean-field laser equations]

We will focus on the second scenario, where the interaction Hamiltonian couples mean collective variables of the system to the environment. The system is described by N copies of the single-particle Hilbert space $\mathcal{H}_S = \mathfrak{h}^{\otimes N}$, and the corresponding N particle Lindblad operator is

$$\mathcal{L}^{(N)} = -i \left[\sum_{i=1}^N h_i, \cdot \right] + \frac{1}{2N} \sum_{i,j=1}^N L_{ij}. \quad (1.40)$$

h_i are identical copies of a self-adjoint single-particle Hamiltonian h . If $i < j$ (respectively, $i > j$), then the L_{ij} are identical copies of the bounded operator L_{12} (respectively, L_{21}) acting on $S(\mathfrak{h} \otimes \mathfrak{h})$. If $i = j$, then the L_{ij} are identical copies of the bounded operator L_{11} on $S(\mathfrak{h})$.

Theorem 2 from [68] proves that if $V^{(N)}(t)$ is a quantum dynamical semigroup with generator (1.40), then it has the mean-field property

$$\lim_{N \rightarrow \infty} \text{Tr}_{k+1 \dots N} V^{(N)}(t) \rho^{(1)}(0)^{\otimes N} = \rho^{(1)}(t)^{\otimes k}, \quad (1.41)$$

and assuming that the single-particle reduced density matrix $\rho^{(1)}(t)$ is differentiable, it evolves according to the effective nonlinear differential equation

$$\frac{d\rho^{(1)}}{dt} = -i[h, \rho^{(1)}] + L_{11} \rho^{(1)} + \text{Tr}_2 \left[(L_{12} + L_{21})(\rho^{(1)} \otimes \rho^{(1)}) \right]. \quad (1.42)$$

The proof uses the same methods as the proof of the Hermitian mean-field theory based on the BBGKY hierarchy. So, no bounds on the the scaling with N are given.

1.4 Quantum algorithms

Quantum computing is a promising technology that could solve complex computational problems that are not solvable in reasonable time by classical computers. The main strategy is to encode the information into quantum degrees of freedom which can be manipulated via unitary transformations. It is known that quantum evolutions are not in general simulable by classical computers, transforming these evolutions into useful computations leads to the so-called quantum advantage. State-of-the art experiments on quantum systems allow one to have control of the individual degrees of freedom making possible to use different platforms as quantum computers. There are many proposals as physical platforms to implement this technology: photons [69], ions [70], neutral atoms [71], molecules [72] and superconducting circuits [73, 74]. There are still many challenges on the physical implementation, the available technology at the moment is called Noisy Intermediate-Scale Quantum (NISQ) computing, but a lot of progress has been done towards the development of fault-tolerant quantum computers.

Once the fault-tolerant stage is reached, one can consider all these physical platforms equivalent and develop algorithms where the main components are qubits, gates and measurements. This abstract construction of algorithms allows the theoretical research to be independent from the physical platform. The main reference as an introduction to the subject is [75]. Next, we will review the main algorithms that we are going to refer to during the thesis.

1.4.1 Hamiltonian simulation and linear systems

The first proposal for quantum advantage was given by Feynman [76], he realized that if we want to simulate a quantum evolution efficiently, we must use quantum computers. This area is called quantum simulation or Hamiltonian simulation algorithms. Given a Hamiltonian H , one encode the initial quantum state $|x_0\rangle$ in the language of qubits and implement a series of gates that implement the unitary evolution such that at the end of the protocol the state is transformed into $|x_t\rangle = e^{-iHt}|x_0\rangle$. Depending on the assumptions on the Hamiltonian, many techniques have been developed [34, 36, 77–83]. We will make use of [84, 85], where they show that, assuming $H \in \mathbb{C}^{d \times d}$ is s -sparse, one can implement the unitary evolution at finite time $t > 0$ given by e^{-iHt} up to error $\epsilon > 0$ with a number $\mathcal{O}(st \max_{i,j} |H_{i,j}| + \frac{\ln(1/\epsilon')}{\ln \ln(1/\epsilon')})$ of queries to the matrix elements of H and additional $\mathcal{O}((\ln d) st \max_{i,j} |H_{i,j}| + \frac{(\ln d) \ln(1/\epsilon')}{\ln \ln(1/\epsilon')})$ one- and two-qubit gates.

This technique is used to simulate linear Schrödinger equations, however, in principle the only restriction is that H should be Hermitian, so we are not restricted to physical

systems but any Schrödinger equation in a finite dimensional Hilbert space with Hermitian generator can be solved in a running time that scales logarithmically in the dimension of the Hilbert space, while classical algorithms can run this simulation in a running time that scales linearly in the dimension of the Hilbert space.

Another relevant problem that can be solved in a quantum computer with exponential advantage is the solution of linear equations. The inputs of a linear problem are a vector $\mathbf{b} \in \mathbb{C}^d$ with components b_j , $j = 0, \dots, d-1$ and a matrix $A \in \mathbb{C}^{d \times d}$ with components $A_{i,j}$, eigenvectors $\mathbf{u}_j$ and eigenvalues λ_j , $i, j = 0, \dots, d-1$. The output is a vector $\mathbf{x} \in \mathbb{C}^d$ satisfying

$$A \cdot \mathbf{x} = \mathbf{b}. \quad (1.43)$$

We focus on s -sparse matrices, namely matrices with a maximum number s of non-vanishing elements in each row or column. Furthermore, we assume the matrix is Hermitian and define the condition number as $\kappa = \max_j |\lambda_j| / \min_j |\lambda_j|$. If the matrix is not Hermitian the problem can be mapped to an equivalent problem with an Hermitian matrix. Consider indeed the following problem

$$\begin{pmatrix} 0 & A \\ A^\dagger & 0 \end{pmatrix} \cdot \mathbf{y} = \begin{pmatrix} \mathbf{b} \\ \mathbf{0} \end{pmatrix}, \quad (1.44)$$

whose solution is the solution of the original problem embedded in $\mathbb{C}^{2d}$: $\mathbf{y} = \mathbf{0} \oplus A^{-1}\mathbf{b} = \mathbf{0} \oplus \mathbf{x}$ where $\mathbf{0} \in \mathbb{C}^d$ is the vector with all components set to zero. Solving the new problem, then solves the original problem at the cost of doubling the dimension of the solution space. This requires only one extra qubit and the condition number of this new matrix is the ratio of the maximum and minimum singular value of A . Finally, assume without loss of generality that the eigenvalues of A satisfy $0 < \lambda_j \leq 1$. The conditions $\lambda_j \leq 1$ can be achieved by dividing A and multiplying $\mathbf{x}$ by a rough estimate (rounded up) of the largest eigenvalue of A . We will show in section 4.5 how to relax the condition $\lambda_j > 0$. The other relevant parameter is ϵ , defined as the tolerated error of the output.

The first quantum algorithm for linear systems was proposed by Harrow, Hassidim and Lloyd [37] (henceforth *HHL algorithm*), although more recent algorithms have been studied and reviewed in [86]. Algorithms based on the adiabatic theorem [87, 88] and eigenstates filtering [89] reach optimal scaling $\mathcal{O}(\kappa \ln(1/\epsilon))$ for the number of queries to matrix elements of A . Other algorithms, relying on quantum singular value transformation [90, 91], exhibit the scaling $\mathcal{O}(\kappa^2 \ln(\kappa/\epsilon))$. These recent algorithms employ the so-called block encoding technique that may require large time or memory [91–93]. Therefore, although the HHL algorithm shows a non-optimal scaling $\mathcal{O}(\kappa^2/\epsilon)$, it remains relevant not only for its conceptual simplicity but also for the simpler implementation with noisy intermediate-scale quantum (NISQ) technologies [94, 95] compared to other algorithms.

The *HHL algorithm* is based on two protocols, the quantum phase estimation [75, 96–98] and the amplitude amplification [99] (a variant of the Grover’s search algorithm [100–102]) that represent the core of general quantum algorithms (solving the so-called BQP-complete problems) [103]. In the original algorithm [37], the quantum phase estimation

is initialized with a complex state that minimizes the final error. A variant of the *HHL algorithm* employing a much simpler initial state (i.e., prepared using Hadamard gates) is often discussed in the literature as it enables experimental implementations with currently available quantum hardware [104–108]. In the following, we refer to this version of the *HHL algorithm* as *HHL variant*.

The algorithm is based on the following observation, the linear problem (1.43) has a solution if and only if $\mathbf{b}$ lies in the support of A . In this case, given the eigenvectors $\mathbf{u}_j$ of A with eigenvalues $\lambda_j \neq 0$, there is a decomposition of the input vector $\mathbf{b} = \sum_j \beta_j \mathbf{u}_j$ for some $\beta_j \in \mathbb{C}$ and the solution is

$$\mathbf{x} = \sum_j (\beta_j / \lambda_j) \mathbf{u}_j. \quad (1.45)$$

An alternative decomposition of the input state is $\mathbf{b} = \sum_j b_j \mathbf{e}_j$, where $\mathbf{e}_j$ are basis vectors with elements $(\mathbf{e}_j)_l = \delta_{j,l}$.

For later convenience, assume that $\mathbf{b}$ has unit L^2 -norm, $\|\mathbf{b}\|_2 = 1$. If this condition is not met, the linear problem (1.43) can be mapped to an equivalent problem by dividing $\mathbf{b}$ and $\mathbf{x}$ by the norm $\|\mathbf{b}\|_2$.

The *HHL algorithm* and its variant use three quantum registers.

- The register r consists of $n = \lceil \log_2 d \rceil$ qubits used to encode the vector $\mathbf{b}$ (padded with zeros if needed) in the pure state $|b\rangle_r = \sum_{j=0}^{d-1} b_j |j\rangle_r$, where $\{|j\rangle_r\}_{j=0,\dots,2^n-1}$ is the computational basis. This is the reason for requiring $1 = \|\mathbf{b}\|_2^2 = \langle b|b \rangle$. This pure state can also be expressed as $|b\rangle_r = \sum_j \beta_j |u_j\rangle_r$, where $|u_j\rangle_r = \sum_k V_{k,j} |k\rangle_r$ and $V = [V_{k,j}]$ is the unitary matrix that diagonalizes A , $V^\dagger A V = \text{diag}(\lambda_1, \dots, \lambda_d)$. The space $\mathbb{C}^d$, where the vectors $\mathbf{x}$ and $\mathbf{b}$ lie, is then encoded in a subspace of the Hilbert space of the register r , that is the span of the n -qubit states $\{|j\rangle_r\}_{j=0,\dots,2^n-1}$ and has dimension $2^n \geq d$ compatibly with $n = \lceil \log_2 d \rceil$.
- The register c , called *clock*, is used to implement the quantum phase estimation and to store the binary representation of eigenvalues of A as elements of the computational basis. It consists of n_c qubits, so that the states in the computational basis represent up to $T = 2^{n_c}$ different values and consequently the maximum precision for eigenvalue estimations is $2^{-n_c} = T^{-1}$. When n_c and T increase, the eigenvalues of A are discriminated with better precision leading to a smaller error in the final output. For this reason, we use T as the parameter to analyse the convergence towards the exact solution.
- The algorithm also uses an additional ancillary qubit a , which is used as a flag to identify the success of the computation.

The solution $\mathbf{x}$ is encoded in the amplitudes of the output state vector of the r -register. Nevertheless, it is impossible to generate a state whose amplitudes are the components of

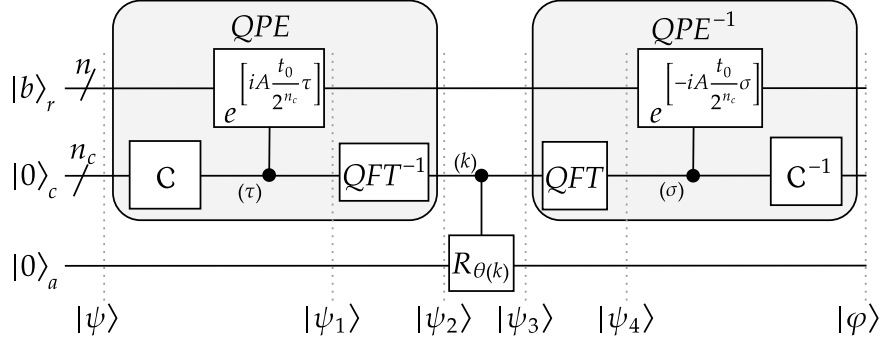


Figure 1.1: Circuit of the main part of the HHL algorithm and of its variant. The first three operators implement the phase estimation protocol. The operation $\mathcal{C}$ represents the preparation of the *clock*, it can be chosen as in (1.47) to implement the original algorithm or as in (1.48) to implement its variant. The notations (τ) , (k) and (σ) indicate controlled operations conditioned on the computational basis states $|\tau\rangle_c$, $|k\rangle_c$ and $|\sigma\rangle_c$ of the c -register respectively. The angle of the rotation $R_{\theta(k)}$ are defined by $\sin \theta(k) := Ct_0/(2\pi k)$. The last three steps uncompute the phase estimation.

$\mathbf{x}$, namely $\sum_j x_j |u_j\rangle_r$ with $x_j = \beta_j/\lambda_j$, because it is not normalized in general. Instead, the HHL algorithm aims at producing a state as close as possible to $\sum_j x_j |u_j\rangle_r / \|\mathbf{x}\|_2$. Unfortunately, the amplitudes can be precisely measured with state tomography which is not efficient in the worst case [109–112]. Therefore, the HHL algorithm does not compute the exact solution $\mathbf{x}$, but it can be used to compute the norm $\|\mathbf{x}\|_2$ and expectation values $\mathbf{x}^\dagger M \mathbf{x}$ of matrices M that can be implemented efficiently on the quantum register.

The main part of the original *HHL algorithm* [37] and of its variant [104–108, 113] is compactly described by the circuit in Figure 1.1. The explicit formulas of intermediate states are reported in section A.1. The quantum registers are initially prepared in the following state

$$|\psi\rangle = |0\rangle_a |0\rangle_c \sum_j \beta_j |u_j\rangle_r. \quad (1.46)$$

The difference between the *HHL algorithm* and its variant is the first operation, $\mathcal{C}$, applied to the clock register, respectively

$$\mathcal{C}^{\text{HHL}} |0\rangle_c = \sqrt{\frac{2}{T}} \sum_{\tau=0}^{T-1} \sin\left(\frac{\pi(2\tau+1)}{2T}\right) |\tau\rangle_c, \quad (1.47)$$

$$\mathcal{C}^{\text{var}} |0\rangle_c = \frac{1}{\sqrt{T}} \sum_{\tau=0}^{T-1} |\tau\rangle_c, \quad (1.48)$$

In the *HHL variant*, the operator $\mathcal{C}^{\text{var}}$ is the Hadamard gate on each qubit of the clock

$|\gamma\rangle_c \rightarrow H^{\otimes n_c} |\gamma\rangle_c = \frac{1}{\sqrt{T}} \sum_{\sigma=0}^{T-1} \exp(i\pi \sum_{l=1}^{n_c} \gamma_l \sigma_l) |\sigma\rangle_c$ with $\{\gamma_l\}_l$ and $\{\sigma_l\}_l$ the binary representations of γ and σ . Therefore, these Hadamard gates can be parallelized such that they require constant time, and the state $\mathcal{C}^{\text{var}}|0\rangle_c$ is fully factorized. The operator $\mathcal{C}^{\text{HHL}}$ in the *HHL algorithm* is more complicated as it entangles the clock qubits, and can be implemented in time $\mathcal{O}(n_c) = \mathcal{O}(\log_2 T)$ [114, 115]. Although the variant slightly reduces circuit complexity, this simplification significantly lowers the precision of the eigenvalue estimation. The initial state of the r -register can be prepared following known state preparation schemes [114–125], or may result from a previous quantum protocol.

In Figure 1.1, we have denoted by QFT the quantum Fourier transform

$$|\tau\rangle_c \rightarrow \frac{1}{\sqrt{T}} \sum_{k=0}^{T-1} e^{-i2\pi\tau k/T} |k\rangle_c, \quad (1.49)$$

and by QFT^{-1} its inverse. The other gates are controlled unitaries defined by the following state transformations

$$|\tau\rangle_c |b\rangle_r \longrightarrow |\tau\rangle_c e^{iA \frac{t_0}{T} \tau} |b\rangle_r, \quad (1.50)$$

$$|0\rangle_a |k\rangle_c \longrightarrow \begin{cases} \sin(\theta(k)) |1\rangle_a |k\rangle_c + \cos(\theta(k)) |0\rangle_a |k\rangle_c & \text{if } k \geq k_{\min} \\ |0\rangle_a |k\rangle_c & \text{if } k < k_{\min} \end{cases}, \quad (1.51)$$

where t_0 and $k_{\min}$ are free parameters and $\sin(\theta(k)) := Ct_0/(2\pi k)$ with $0 < C \leq 2\pi k_{\min}/t_0$. The implementability of the transformation (1.50) on a quantum computer requires the Hermiticity of A assumed above.

The state vector after these operations for both algorithms is of the form

$$\begin{aligned} |\varphi\rangle &= \frac{1}{\sqrt{T}} \sum_{j=0}^{2^n-1} \sum_{\sigma=0}^{T-1} \sum_{k=k_{\min}}^{T-1} \beta_j \alpha_{k|j} \sin(\theta(k)) e^{i\frac{\sigma}{T}(2\pi k - \lambda_j t_0)} |1\rangle_a \mathcal{C}^{-1} |\sigma\rangle_c |u_j\rangle_r \\ &+ \frac{1}{\sqrt{T}} \sum_{j=0}^{2^n-1} \sum_{\sigma=0}^{T-1} \sum_{k=k_{\min}}^{T-1} \beta_j \alpha_{k|j} \cos(\theta(k)) e^{i\frac{\sigma}{T}(2\pi k - \lambda_j t_0)} |0\rangle_a \mathcal{C}^{-1} |\sigma\rangle_c |u_j\rangle_r \\ &+ \frac{1}{\sqrt{T}} \sum_{j=0}^{2^n-1} \sum_{\sigma=0}^{T-1} \sum_{k=0}^{k_{\min}-1} \beta_j \alpha_{0|j} e^{i\frac{\sigma}{T}(2\pi k - \lambda_j t_0)} |0\rangle_a \mathcal{C}^{-1} |\sigma\rangle_c |u_j\rangle_r, \end{aligned} \quad (1.52)$$

with coefficients

$$\begin{aligned}\alpha_{k|j}^{\text{HHL}} &= \frac{\sqrt{2}}{T} \sum_{\tau=0}^{T-1} e^{i\frac{\tau}{T}(\lambda_j t_0 - 2\pi k)} \sin\left(\frac{\pi(2\tau+1)}{2T}\right) \\ &= e^{i\phi} \frac{\sqrt{2} \cos\left(\frac{1}{2}(\lambda_j t_0 - 2\pi k)\right) \cos\left(\frac{1}{2T}(\lambda_j t_0 - 2\pi k)\right) \sin\left(\frac{\pi}{2T}\right)}{T \sin\left(\frac{1}{2T}(\lambda_j t_0 - 2\pi k + \pi)\right) \sin\left(\frac{1}{2T}(\lambda_j t_0 - 2\pi k - \pi)\right)},\end{aligned}\quad (1.53)$$

$$\alpha_{k|j}^{\text{var}} = \frac{1}{T} \sum_{\tau=0}^{T-1} e^{i\frac{\tau}{T}(\lambda_j t_0 - 2\pi k)} = e^{i\phi} \frac{\sin\left(\frac{1}{2}(\lambda_j t_0 - 2\pi k)\right)}{T \sin\left(\frac{1}{2T}(\lambda_j t_0 - 2\pi k)\right)}, \quad (1.54)$$

for the original *HHL algorithm* and its variant. The phase $\phi = \frac{1}{2}(\lambda_j t_0 - 2\pi k)(1 - \frac{1}{T})$ is not relevant in the following analysis.

The first three operators in Figure 1.1 for the *HHL variant* are the standard quantum phase estimation algorithm (QPE) used to estimate the eigenvalues of A . The operation $\mathcal{C}^{\text{HHL}}$ in the original *HHL algorithm* prepares a state that minimizes the error of the quantum phase estimation [126–128]. The controlled rotations defined in (1.51) implement the inversion of the eigenvalues, requiring the register a to be in the state $|1\rangle_a$ when the inversion succeeds and in $|0\rangle_a$ otherwise. The parameter $k_{\min}$ acts as a cutoff on the spectrum of A . The register state $|k\rangle_c$ encodes the eigenvalue $2\pi k/t_0$, such that the operator (1.51) correctly inverts the eigenvalues bigger than $2\pi k_{\min}/t_0$. Setting the minimum possible value $k_{\min} = 1$ allows one to invert the largest number of eigenvalues, as is typically done in applications of the *HHL variant* [104–108, 113]. If an upper bound of the condition number $\kappa \leq \kappa'$ is available, then we can set $k_{\min} = \lfloor t_0/(4\pi\kappa') \rfloor$. Since the coefficients $\alpha_{k|j}$ are centered around $2\pi k/t_0 \approx \lambda_j$ and recalling $\sin\theta(k) := Ct_0/(2\pi k)$, the coefficients in the first line of equation (1.52) are estimates of the desired coefficients $x_j = \beta_j/\lambda_j$.

The outputs of both the original *HHL algorithm* and its variant are then achieved by measuring the ancillary qubit in the basis $\{|0\rangle_a, |1\rangle_a\}$ and postselecting the outcome 1 which occurs with probability

$$p_0 = \sum_{j=0}^{2^n-1} |\beta_j|^2 \sum_{k=k_{\min}}^{T-1} |\alpha_{k|j}|^2 \left(\frac{C t_0}{2\pi k}\right)^2, \quad (1.55)$$

which can be small. Nevertheless, one can find the outcome $|1\rangle_a$ after applying the amplitude amplification algorithm [99, 102] to the state (1.52) with an average running time $\mathcal{O}(1/\sqrt{p_0})$. The final normalized outputs of the circuits in Figure 1.1 are of the form

$$|x_0\rangle = \frac{1}{\sqrt{T p_0}} \sum_{j=0}^{2^n-1} \sum_{\sigma=0}^{T-1} \sum_{k=k_{\min}}^{T-1} \beta_j \alpha_{k|j} \frac{C t_0}{2\pi k} e^{i\frac{\sigma}{T}(2\pi k - \lambda_j t_0)} |1\rangle_a \mathcal{C}^{-1} |\sigma\rangle_c |u_j\rangle_r, \quad (1.56)$$

with the coefficients (1.53) or (1.54).

The output (1.56) approximates the desired vector $\mathbf{x}/\|\mathbf{x}\|$ with a precision that increases with $T = 2^{n_c}$. In chapter 4 we will compute the convergence rate and we will discuss the optimal choice of parameters C and $k_{\min}$. We will show that the convergence of the *HHL variant* depends on having a bound κ' of the condition number κ . Algorithms for estimating the condition number of an arbitrary sparse matrix are based on the Lanczos algorithm [129], the LU decomposition or the QR decomposition of the matrix A . However, the running time of known algorithms [130–132] has the same scaling with respect to the parameters s and d as classical algorithms that solve linear problems, namely $\mathcal{O}(sd)$ times the number of iterations required in specific algorithms. Therefore, the extension of the HHL algorithm to the case of unknown condition number is relevant as its computation typically negates the advantage of using quantum linear solvers and we will present a new variant whose convergence does not depend on this bound.

1.4.2 Nonlinear differential equation solvers

Since quantum computers present this exponential advantage at solving linear systems, an efficient method to solve nonlinear differential equations is to linearize them in order to obtain an equation that can be treated with the algorithms explained in the last section. We recommend the reader the following review [133] to have an overview of different methods. Lloyd et al. [33] proposed a linearization method based on the mean-field Hartree equation that leads to quantum advantage.

Let $x \in \mathbb{C}^d$ satisfy the nonlinear differential equation

$$\frac{dx}{dt} + f(x)x = b(t), \quad (1.57)$$

where $f(x)$ is a $d \times d$ matrix that is an order m polynomial function of the vectors x and $x^\dagger$, and $b(t) \in \mathbb{C}^d$ is a time dependent vector. They show how to write

$$f(x) = x^{\dagger \otimes m} F x^{\otimes m} \quad (1.58)$$

for some tensor $F \in (\mathbb{C}^{d \times d})^{\otimes m+1}$.

Consider the case where $b(t) = 0$ and f is anti-Hermitian, then F is also anti-Hermitian. One can identify that this equation can be derived from a mean-field system of $N \gg m$ particles with Hamiltonian

$$H = -i \binom{N-1}{m}^{-1} \sum_{1 \leq j_1 \dots j_{m+1} \leq N} F_{j_1 \dots j_{m+1}} \quad (1.59)$$

The derivation of the mean-field equation for Hamiltonians with multi-particle interactions is derived in [134], and it corresponds to the equation (1.57) we want to solve.

Given these observations, the algorithm works as follows. We want to solve the equation

$$\frac{dx}{dt} + (x^{\dagger \otimes m} F x^{\otimes m}) x = 0 \quad (1.60)$$

with initial condition $x_0 \in \mathbb{C}^d$. Assume that $\log_2(d)$ is an integer, otherwise we can pad the vector and the tensor with zeros to have the correct dimension of the vector space. Now we can map the vector x_0 into the state of $\log_2(d)$ qubits $|x_0\rangle$. Initialize $N \gg m$ copies of the initial state into the $N \log_2(d)$ -qubits state $|x_0\rangle^{\otimes N}$. Apply several steps of the Hamiltonian simulation using the Hamiltonian (1.59) for time steps Δt . By the mean-field theory, measurements of single-particle observables on this state would approximate the measurements made on the solution of equation (1.60). For short total evolution times t , the error scales as $\epsilon = \mathcal{O}(t\Delta t m^2/N)$, so it is enough to consider a number of copies that scales quadratically with the order m of the equation and in time. For long time evolutions the accuracy of the simulation depends on the Lyapunov exponents of the nonlinear equation and it is discussed in the article.

The key observation is that N is independent of d . Since the Hamiltonian simulation scales logarithmically in the dimension of the Hilbert space, which is linear in the number of qubits $N \log_2(d)$, the running time is $\mathcal{O}(\log_2(d)t\Delta t m^2/\epsilon)$.

Under the assumption that the mean-field approximation can be generalized to non-Hermitian Hamiltonians, a similar technique could solve the general equation (1.57). The main difficulty is that if the Hamiltonian is not Hermitian, the evolution is not unitary and it is not possible to simulate it in a quantum computer, nonetheless, they proposed to discretize time using standard numerical methods (like Euler forward, Euler backwards, Crank-Nicholson or Runge-Kutta depending on stability requirements) to convert the problem of simulation into an algebraic linear equation. The strategy to get quantum advantage is to solve this linear equation using the HHL algorithm. It allows one to solve this discretized time linear problem in running time logarithmic in the total dimension and thus surpassing the capabilities of classical algorithms for large dimension d .

The results from chapter 2 will show that the assumption that the mean-field approximation can be extended to non-Hermitian Hamiltonians is not justified and indeed it may fail in most of the cases. Also motivated by this proposal, and by the rigorous results presented in subsection 1.3.2, showing that the mean-field approximation holds for open quantum systems, we will show in section 2.5 that any differential equation with polynomial nonlinearity can be written as the mean-field effective equation of an open quantum system. This is the first step into the development of a new algorithm motivated by [33] but replacing the non-Hermitian Schrödinger equation by the GKSL equation.

Chapter 2

Dissipative mean-field systems

In the previous chapter, we discussed how the physics literature, starting from the non-unitary N -body Schrödinger evolution with a non-Hermitian mean-field Hamiltonian, considers the normalized k -particle marginals $\hat{\rho}^{(k)} = \rho^{(k)} / \text{Tr } \rho^{(k)}$, whose dynamics is already nonlinear because of the normalization. Closing the resulting (normalized) BBGKY hierarchy by the usual factorization ansatz for which the few-body marginal states are factorized, i.e., $\hat{\rho}^{(k)} \approx (\hat{\rho}^{(1)})^{\otimes k}$, yields a trace-preserving nonlinear evolution equation for $\hat{\rho}^{(1)}$ in the thermodynamic limit. Applications of the corresponding equation are described in subsection 1.3.1 and subsection 1.4.2.

The main message of the chapter is that, even for extremely simple Hamiltonians, the non-Hermitian Hartree equation can fail to capture the one-particle dynamics. In section 2.1, we present a general discussion on the mean-field approximation with non-Hermitian Hamiltonians, showing how the BBGKY hierarchy is modified, and by analyzing the second time derivative at the initial time, we derive a necessary condition for the success of the mean-field approximation relating the non-Hermitian Hamiltonian and the initial condition. In section 2.2, we provide an explicit, exactly solvable counterexample: a bosonic system of N qubits with two-particle interactions generated by a *purely anti-Hermitian* Hamiltonian. For any factorized initial wavefunction in the completely symmetric subspace, we compute the exact normalized one-particle marginal state $\hat{\rho}_N^{(1)}(t)$ and compare its limit as $N \rightarrow \infty$ with the solution of the non-Hermitian Hartree equation. Our analytical large- N analysis and supporting numerics show:

- **Persistent failure of the Hartree approximation:** For almost any initial condition, the limit as $N \rightarrow \infty$ of the one-particle marginal state is pure but different from the solution of the non-Hermitian Hartree equation. Indeed, such a limit is governed by an effective evolution equation that depends explicitly on time and agrees with the Hartree equation only at $t = 0$.
- **Finite-time mixedness transition:** There exists an initial condition for which the limit as $N \rightarrow \infty$ of the one-particle marginal state undergoes a sharp transition

from a pure state to a mixed state at a finite critical time, a phenomenon which is completely absent for Hermitian Hamiltonians and is indicative of correlations that survive the mean-field limit.

In order to complement this example, we numerically solve two other bosonic systems of N qubits. In section 2.3, we consider a Hamiltonian with two-body interactions having a real spectrum, and in section 2.4, we consider a Hamiltonian with only single-particle operators, but where the initial state is in a condensate that is not an exact product state. The numerical solutions confirm the observations made in the first example.

Our counterexamples highlight that non-unitarity can amplify correlations in a way that prevents the usual mean-field closure. This suggests that approximating bosonic many-body non-Hermitian systems by an effective Hartree equation, as in subsection 1.4.2, may require extra justification, rather than being taken as a generic consequence of large N . As an alternative to the algorithm [33], we propose that one can embed the nonlinear equation into an open quantum system. In section 2.5, we provide a first step in this direction by proving that if the Hartree approximation holds for the Lindblad evolution in the mean-field regime, then any equation with polynomial nonlinearity can be obtained as a Hartree equation of an open quantum system.

2.1 The Hartree equation for non-Hermitian Hamiltonians

Let $\mathfrak{h}$ be the Hilbert space of a single particle, which we assume to have finite dimension, and let $\text{Sym}^N \mathfrak{h}$ be its N -fold symmetrized tensor product. Mean-field Hamiltonians are constructed by a one-particle operator $A^{(1)}$ acting on $\mathfrak{h}$ and a two-particle operator $A^{(2)}$ acting on $\mathfrak{h}^{\otimes 2}$ and invariant with respect to the swap of the two particles. The N -particle mean-field non-Hermitian Hamiltonian $A^{(N)}$ is

$$A^{(N)} = \sum_{i=1}^N A_i^{(1)} + \frac{1}{N-1} \sum_{1 \leq i < j \leq N} A_{ij}^{(2)}, \quad (2.1)$$

where subscripts indicate on which particles the one-particle and the two-particle operators act. We stress that $A^{(N)}$ is invariant with respect to arbitrary permutations of the particles and therefore leaves the completely symmetric subspace $\text{Sym}^N \mathfrak{h}$ invariant.

Let us consider the non-Hermitian Schrödinger equation

$$\begin{cases} i\partial_t \Psi^{(N)} = A^{(N)} \Psi^{(N)} \\ \Psi^{(N)}(0) = \varphi^{\otimes N}, \end{cases} \quad (2.2)$$

for the N -particle wavefunction $\Psi^{(N)} \in \mathfrak{h}^{\otimes N}$, where the initial condition is a factorized wavefunction in which each particle is in the state $\varphi \in \mathfrak{h}$. Without loss of generality, we

assume that $\|\varphi\| = 1$. Equation (2.2) can also be written in terms of the unnormalized N -particle state $\rho^{(N)} := |\Psi^{(N)}\rangle\langle\Psi^{(N)}|$,

$$\begin{cases} i\partial_t \rho^{(N)} = A^{(N)} \rho^{(N)} - \rho^{(N)} A^{(N)\dagger} \\ \rho^{(N)}(0) = |\varphi\rangle\langle\varphi|^{\otimes N}. \end{cases} \quad (2.3)$$

For any $k = 1, \dots, N-1$, the unnormalized k -particle marginal state is defined by

$$\rho^{(k)} = \text{Tr}_{k+1\dots N} \rho^{(N)}. \quad (2.4)$$

This definition implies the normalization

$$\text{Tr} \rho^{(k)} = \text{Tr} \rho^{(N)} = \|\Psi^{(N)}\|^2 \quad \forall k = 1, \dots, N-1, \quad (2.5)$$

where the norm of $\Psi^{(N)}$ can change in time because the evolution is not unitary. The evolution equation for the unnormalized one-particle marginal state is computed by taking the partial trace of equation (2.3):

$$\begin{aligned} i\partial_t \rho^{(1)} = & A^{(1)} \rho^{(1)} - \rho^{(1)} A^{(1)\dagger} + \text{Tr}_2 \left(A^{(2)} \rho^{(2)} - \rho^{(2)} A^{(2)\dagger} \right) \\ & + (N-1) \text{Tr}_2 \left(\left(\mathbb{I} \otimes \left(A^{(1)} - A^{(1)\dagger} \right) \right) \rho^{(2)} \right) \\ & + \frac{N-2}{2} \text{Tr}_{23} \left(\left(\mathbb{I} \otimes \left(A^{(2)} - A^{(2)\dagger} \right) \right) \rho^{(3)} \right). \end{aligned} \quad (2.6)$$

For any $k = 1, \dots, N$, let

$$\hat{\rho}^{(k)} = \frac{\rho^{(k)}}{\text{Tr} \rho^{(k)}} \quad (2.7)$$

be the normalized k -particle marginal state, which will simply be called k -particle marginal state. The evolution equation for the one-particle marginal state is

$$\begin{aligned} i\partial_t \hat{\rho}^{(1)} = & A^{(1)} \hat{\rho}^{(1)} - \hat{\rho}^{(1)} A^{(1)\dagger} - \text{Tr} \left(\left(A^{(1)} - A^{(1)\dagger} \right) \hat{\rho}^{(1)} \right) \hat{\rho}^{(1)} \\ & + \text{Tr}_2 \left(A^{(2)} \hat{\rho}^{(2)} - \hat{\rho}^{(2)} A^{(2)\dagger} \right) - \text{Tr} \left(\left(A^{(2)} - A^{(2)\dagger} \right) \hat{\rho}^{(2)} \right) \hat{\rho}^{(1)} \\ & + (N-1) \text{Tr}_2 \left(\left(\mathbb{I} \otimes \left(A^{(1)} - A^{(1)\dagger} \right) \right) \left(\hat{\rho}^{(2)} - \hat{\rho}^{(1)} \otimes \hat{\rho}^{(2)} \right) \right) \\ & + \frac{N-2}{2} \text{Tr}_{23} \left(\left(\mathbb{I} \otimes \left(A^{(2)} - A^{(2)\dagger} \right) \right) \left(\hat{\rho}^{(3)} - \hat{\rho}^{(1)} \otimes \hat{\rho}^{(2)} \right) \right). \end{aligned} \quad (2.8)$$

The first two lines contain the usual terms in the Hartree equation, plus terms that control the norm in the non-Hermitian case. The main novelty in the non-Hermitian case is in the last two lines, where the terms are multiplied by a factor N and vanish in the Hermitian case. To obtain a closed evolution equation for $\hat{\rho}^{(1)}$ from equation (2.8), the heuristic approach that works in the Hermitian case, and followed by [55, 56], is to postulate

that the two-particle marginal state $\hat{\rho}^{(2)}$ approximately remains a product state: $\hat{\rho}^{(2)} \simeq \hat{\rho}^{(1)\otimes 2}$. In the non-Hermitian case, the time derivative of $\hat{\rho}^{(1)}$ depends also on the three-particle marginal state $\hat{\rho}^{(3)}$. Therefore, we will obtain the nonlinear Schrödinger equation by postulating that also the three-particle state remains a product state: $\hat{\rho}^{(3)} \simeq \hat{\rho}^{(1)\otimes 3}$. Assuming that all these postulates hold true and replacing $\hat{\rho}^{(k)}$ by $\gamma^{\otimes k}$ in equation (2.8) for $k = 1, 2, 3$ gives the following non-Hermitian Hartree equation:

$$\begin{aligned} i\partial_t \gamma &= A^{(1)}\gamma - \gamma A^{(1)\dagger} - \text{Tr} \left(\left(A^{(1)} - A^{(1)\dagger} \right) \gamma \right) \gamma \\ &\quad + \text{Tr}_2 \left(A^{(2)} (\mathbb{I} \otimes \gamma) \right) \gamma - \gamma \text{Tr}_2 \left((\mathbb{I} \otimes \gamma) A^{(2)\dagger} \right) \\ &\quad - \text{Tr} \left(\left(A^{(2)} - A^{(2)\dagger} \right) \gamma^{\otimes 2} \right) \gamma, \end{aligned} \quad (2.9)$$

with initial condition $\gamma(0) = |\varphi\rangle\langle\varphi|$. We claim that γ will be pure and normalized at any time. Indeed, $\gamma = |\phi\rangle\langle\phi|$ satisfies (2.9) if the Hartree wavefunction $\phi \in \mathfrak{h}$ satisfies the non-Hermitian nonlinear Schrödinger equation

$$i\partial_t \phi = \left(A^{(1)} - \left\langle \phi, \frac{A^{(1)} - A^{(1)\dagger}}{2} \phi \right\rangle + \left\langle \phi, A^{(2)} \phi \right\rangle - \left\langle \phi^{\otimes 2}, \frac{A^{(2)} - A^{(2)\dagger}}{2} \phi^{\otimes 2} \right\rangle \right) \phi, \quad (2.10)$$

with initial condition $\phi(0) = \varphi$. Furthermore, the solution of (2.10) has unit norm at any time.

We will analyze two quantities related to the Hartree approximation. The linear entropy is defined as

$$S_L := 1 - \text{Tr} \hat{\rho}^{(1)2}, \quad (2.11)$$

and quantifies the closeness of $\rho^{(1)}$ to a pure state. If $S_L \approx 0$, the one-particle marginal state is approximately pure, which implies that the k -particle marginal states can be approximated by a product state for any finite k : $\hat{\rho}^{(k)} \approx \hat{\rho}^{(1)\otimes k}$ for large N . Then, we define the infidelity with respect to the solution of the Hartree equation as

$$I := 1 - \langle \phi, \hat{\rho}^{(1)} \phi \rangle, \quad (2.12)$$

which measures whether such a solution correctly describes the one-particle marginal state of the solution of the corresponding many-body dynamics.

The case where $A^{(2)} = 0$ and the initial condition is a product state is a trivial example where $S_L = 0$ and $I = 0$ at any time. For Hermitian Hamiltonians, it is known [13] that the infidelity with respect to the solution of the Hartree equation scales as N^{-1} for a broad family of two-body Hamiltonians. However, we can already observe from equation (2.8) that the last two terms depending on the anti-Hermitian part of the Hamiltonian have a prefactor $\mathcal{O}(N)$. Therefore, even in the case where $\hat{\rho}^{(2)} = \hat{\rho}^{(1)\otimes 2} + \mathcal{O}(N^{-1})$, the non-Hermitian terms in the Hamiltonian will generate corrections to the Hartree equation that remain finite in the limit $N \rightarrow \infty$. Consequently, in the limit $N \rightarrow \infty$, the evolution of $\hat{\rho}^{(1)}$

will depend on $\hat{\rho}^{(2)}$ and $\hat{\rho}^{(3)}$, and this is not captured by the Hartree equation. In the next subsection, we will show how this amplification due to the anti-Hermitian terms works at short times.

2.1.1 Short-time behavior of the reduced one-particle state

In this subsection, we compare the first and second time derivatives at $t = 0$ of the solution of the Hartree equation (2.9) and of the exact one-particle reduced density matrix (2.8). We will show that, even when the initial state is a product state, the Hartree approximation captures the correct first time derivative but fails to describe the second time derivative. This deviation is only present for Hamiltonians that are not Hermitian and contain interaction terms.

The first derivatives of γ and of $\hat{\rho}^{(1)}$ are given by the Hartree equation (2.9) and by the hierarchy (2.8), respectively. Observe that at $t = 0$, since $\hat{\rho}^{(1)}(0) = \gamma(0) = |\varphi\rangle\langle\varphi|$, and furthermore since $\hat{\rho}^{(k)}(0) = \gamma(0)^{\otimes k}$, both expressions match:

$$i\partial_t\gamma|_{t=0} = i\partial_t\hat{\rho}^{(1)}|_{t=0}. \quad (2.13)$$

This is true by construction, because the last two terms in (2.8), scaling with N , cancel exactly.

Let us now consider the first time derivative of the k -particle reduced density matrices. By taking the partial trace of the evolution equation (2.3) over the last $N - k$ particles, we can compute the evolution equation of the k -particle reduced density matrix. One can then normalize it and, proceeding as in the derivation of (2.8), we get the following evolution equation:

$$\begin{aligned} i\partial_t\hat{\rho}^{(k)} &= \sum_{i=1}^k \left(A_i^{(1)} - \text{Tr} \left(A^{(1)}\hat{\rho}^{(1)} \right) \right) \hat{\rho}^{(k)} - h.c. \\ &+ \frac{N-k}{N-1} \sum_{i=1}^k \text{Tr}_{k+1} \left(\left(A^{(2)} - \text{Tr} \left(A^{(2)}\hat{\rho}^{(2)} \right) \right)_{i,k+1} \hat{\rho}^{(k+1)} \right) - h.c. \\ &+ (N-k) \text{Tr}_{k+1} \left(G_{k+1}^{(1)} \left(\hat{\rho}^{(k+1)} - \hat{\rho}^{(k)} \otimes \hat{\rho}^{(1)} \right) \right) \\ &+ \frac{1}{N-1} \binom{N-k}{2} \text{Tr}_{k+1,k+2} \left(G_{k+1,k+2}^{(2)} \left(\hat{\rho}^{(k+2)} - \hat{\rho}^{(k)} \otimes \hat{\rho}^{(2)} \right) \right) \\ &+ \frac{1}{N-1} \sum_{1 \leq i < j \leq k} \left(A^{(2)} - \text{Tr} \left(A^{(2)}\hat{\rho}^{(2)} \right) \right)_{ij} \hat{\rho}^{(k)} - h.c.. \end{aligned} \quad (2.14)$$

In order to simplify notation, we define $G^{(i)} = A^{(i)} - A^{(i)\dagger}$ for $i = 1, 2$, we use sub indexes to indicate the particle where an operator acts and we write $h.c.$ for Hermitian conjugate. At time $t = 0$, using that $\rho^{(k)}(0) = \gamma(0)^{\otimes k}$, the time derivative simplifies to

$$\begin{aligned}
i\partial_t \hat{\rho}^{(k)}|_{t=0} &= \sum_{i=1}^k \left(A_i^{(1)} - \text{Tr} \left(A^{(1)} \gamma(0) \right) \right) \gamma(0)^{\otimes k} - h.c. \\
&+ \frac{N-k}{N-1} \sum_{i=1}^k \text{Tr}_{k+1} \left(\left(A^{(2)} + \text{Tr} \left(A^{(2)} \gamma(0)^{\otimes 2} \right) \right)_{i,k+1} \gamma(0)^{\otimes k+1} \right) - h.c. \\
&+ \frac{1}{N-1} \sum_{1 \leq i < j \leq k} \left(A^{(2)} - \text{Tr} \left(A^{(2)} \gamma(0)^{\otimes 2} \right) \right)_{ij} \gamma(0)^{\otimes k} - h.c. .
\end{aligned} \tag{2.15}$$

On the other hand, using the Hartree equation, one gets the time derivative

$$\begin{aligned}
i\partial_t \gamma^{\otimes k} &= \sum_{i=1}^k \left(A^{(1)} - \text{Tr} \left(A^{(1)} \gamma \right) \right)_i \gamma^{\otimes k} - h.c. \\
&+ \sum_{i=1}^k \text{Tr}_{k+1} \left(\left(A^{(2)} + \text{Tr} \left(A^{(2)} \gamma^{\otimes 2} \right) \right)_{i,k+1} \gamma^{\otimes k+1} \right) - h.c. .
\end{aligned} \tag{2.16}$$

Comparing (2.15) and (2.16), we can see that

$$i\partial_t \hat{\rho}^{(k)}|_{t=0} = i\partial_t \gamma^{\otimes k}|_{t=0} + \mathcal{O}\left(\frac{k}{N}\right). \tag{2.17}$$

Then, for any fixed k , in the limit of a large number of particles the Hartree equation describes correctly the first time derivative of $\hat{\rho}^{(k)}$. However, it is important to observe that the approximation error is $\mathcal{O}(N^{-1})$, because the next step is to compute the second derivative, and we will show that these small corrections are amplified in the non-Hermitian case and lead to a finite difference between the second derivative of the exact one-particle reduced density matrix and of the Hartree solution. Taking the time derivative of (2.9) one gets the second time derivative of the Hartree solution:

$$\begin{aligned}
-\partial_t^2 \gamma &= \left(A^{(1)} - \text{Tr} \left(A^{(1)} \gamma \right) \right) i\partial_t \gamma - \text{Tr} \left(A^{(1)} i\partial_t \gamma \right) \gamma - h.c. \\
&+ \text{Tr}_2 \left(\left(A^{(2)} - \text{Tr} \left(A^{(2)} \gamma^{\otimes 2} \right) \right) i\partial_t \gamma^{\otimes 2} \right) - \text{Tr} \left(A^{(2)} i\partial_t \gamma^{\otimes 2} \right) \gamma - h.c. .
\end{aligned} \tag{2.18}$$

We compute the second time derivative of the one-particle reduced density matrix by taking the time derivative of (2.8):

$$\begin{aligned}
-\partial_t^2 \hat{\rho}^{(1)} &= \left(A^{(1)} - \text{Tr} \left(A^{(1)} \hat{\rho}^{(1)} \right) \right) i\partial_t \hat{\rho}^{(1)} - \text{Tr} \left(A^{(1)} i\partial_t \hat{\rho}^{(1)} \right) \hat{\rho}^{(1)} + h.c. \\
&+ \text{Tr}_2 \left(\left(A^{(2)} - \text{Tr} \left(A^{(2)} \hat{\rho}^{(2)} \right) \right) i\partial_t \hat{\rho}^{(2)} \right) - \text{Tr} \left(A^{(2)} i\partial_t \hat{\rho}^{(2)} \right) \hat{\rho}^{(1)} + h.c. \\
&+ (N-1) \text{Tr}_2 \left(G_2^{(1)} \left(i\partial_t \hat{\rho}^{(2)} - i\partial_t \hat{\rho}^{(1)} \otimes \hat{\rho}^{(1)} - \hat{\rho}^{(1)} \otimes i\partial_t \hat{\rho}^{(1)} \right) \right) \\
&+ \frac{N-2}{2} \text{Tr}_{23} \left(G_{23}^{(2)} \left(i\partial_t \hat{\rho}^{(3)} - i\partial_t \hat{\rho}^{(1)} \otimes \hat{\rho}^{(2)} - \hat{\rho}^{(1)} \otimes i\partial_t \hat{\rho}^{(2)} \right) \right) .
\end{aligned} \tag{2.19}$$

Using the previous results (2.13) and (2.17), it follows that the first two lines in (2.19) are reproduced by (2.18) at the initial time up to small corrections $\mathcal{O}(N^{-1})$. Now we will compute the last two lines and show that they contribute with extra terms which modify the second time derivative.

Let us use (2.15) with $k = 1, 2$, to compute

$$\begin{aligned} & \left(i\partial_t \hat{\rho}^{(2)} - i\partial_t \hat{\rho}^{(1)} \otimes \hat{\rho}^{(1)} - \hat{\rho}^{(1)} \otimes i\partial_t \hat{\rho}^{(1)} \right) \Big|_{t=0} = \\ & - \frac{1}{N-1} \sum_{i=1}^2 \text{Tr}_3 \left(\left(A^{(2)} - \text{Tr} \left(A^{(2)} \gamma(0)^{\otimes 2} \right) \right)_{i,3} \gamma(0)^{\otimes 3} \right) \\ & + \frac{1}{N-1} \left(A^{(2)} - \text{Tr} \left(A^{(2)} \gamma(0)^{\otimes 2} \right) \right) \gamma(0)^{\otimes 2} - h.c.. \end{aligned} \quad (2.20)$$

Similarly, we can use (2.15) with $k = 1, 2, 3$ to compute

$$\begin{aligned} & \left(i\partial_t \hat{\rho}^{(3)} - i\partial_t \hat{\rho}^{(1)} \otimes \hat{\rho}^{(2)} - \hat{\rho}^{(1)} \otimes i\partial_t \hat{\rho}^{(2)} \right) \Big|_{t=0} = \\ & - \frac{1}{N-1} \sum_{i=2}^3 \text{Tr}_4 \left(\left(A^{(2)} - \text{Tr} \left(A^{(2)} \gamma(0)^{\otimes 2} \right) \right)_{i,4} \gamma(0)^{\otimes 4} \right) \\ & - \frac{2}{N-1} \text{Tr}_4 \left(\left(A^{(2)} - \text{Tr} \left(A^{(2)} \gamma(0)^{\otimes 2} \right) \right)_{14} \gamma(0)^{\otimes 4} \right) \\ & + \frac{1}{N-1} \sum_{i=2}^3 \left(A^{(2)} - \text{Tr} \left(A^{(2)} \gamma(0)^{\otimes 2} \right) \right)_{1i} \gamma(0)^{\otimes 3}. \end{aligned} \quad (2.21)$$

Plugging the expressions (2.20) and (2.21) into (2.19), subtracting the second derivative of the Hartree equation at time $t = 0$ and using the properties of the partial trace, we get

$$\begin{aligned} -\partial_t^2 (\hat{\rho}^{(1)} - \gamma)|_{t=0} &= \left[\text{Tr}_2 \left(\left(G^{(1)} - \text{Tr} \left(G^{(1)} \gamma(0) \right) \right)_2 A^{(2)} \gamma(0)_2 \right) \right. \\ & \quad \left. - \text{Tr} \left(G_2^{(1)} \left(A^{(2)} - \text{Tr} \left(A^{(2)} \gamma(0)^{\otimes 2} \right) \right) \gamma(0)^{\otimes 2} \right) \right] \gamma(0) + h.c. \\ & + \left[\text{Tr}_{23} \left(\left(G^{(2)} - \text{Tr} \left(G^{(2)} \gamma(0)^{\otimes 2} \right) \right)_{23} A_{12}^{(2)} \gamma(0)_2 \gamma(0)_3 \right) \right. \\ & \quad \left. - \text{Tr} \left(G_{23}^{(2)} \left(A^{(2)} - \text{Tr} \left(A^{(2)} \gamma(0)^{\otimes 2} \right) \right)_{12} \gamma^{\otimes 3} \right) \right] \gamma(0) + h.c. \\ & + \mathcal{O} \left(\frac{1}{N} \right). \end{aligned} \quad (2.22)$$

The conclusion of this computation is that the Hartree equation is constructed in such a way that at $t = 0$, when the system is exactly in a product state, the first time derivative

of the Hartree solution and of the exact one-particle reduced density matrix are the same, and this is shown in (2.13). The same construction shows that for any fixed k , the difference between the time derivative of k copies of the Hartree solution and the k -particle reduced density matrix vanishes for large N with an error of order $\mathcal{O}(N^{-1})$ as shown in (2.17). Even if the first time derivative matches, the difference between the second derivative of the one-particle reduced density matrix and of the Hartree solution has contributions that do not vanish for large N , and this is shown in (2.22). These contributions are present only on the non-Hermitian case, since they depend on the anti-Hermitian Hamiltonian terms $G^{(i)}$, $i = 1, 2$ and furthermore they also vanish if there is no interaction, i.e., if $A^{(2)} = 0$. This shows how the non-Hermitian terms of the Hamiltonian amplify the approximation error of the mean-field approximation in such a way that even at small times, the difference between the Hartree solution and the exact one-particle reduced density matrix does not vanish.

Furthermore, assuming that the large N limit commutes with the time derivative, given a non-Hermitian Hamiltonian, it is a necessary condition on the initial state for the success of the Hartree approximation that $\lim_{N \rightarrow \infty} \partial_t^2 (\hat{\rho}^{(1)} - \gamma) |_{t=0} = 0$. We will show that asking for the r.h.s of (2.22) to vanish in the large N limit is a very restrictive condition when applied to the different examples in subsection 2.2.3 and subsection 2.3.3.

2.2 ZZ anti-Hermitian interaction

We present a nontrivial example in which the solution of the non-Hermitian nonlinear Schrödinger equation (2.9) and the limit for $N \rightarrow \infty$ of the one-particle normalized marginal state (2.2) can both be analytically computed and do not agree.

Let each particle be a qubit, since the Hilbert space is $\mathfrak{h} = \mathbb{C}^2 = \text{Span}\{|0\rangle, |1\rangle\}$, we will use the usual bra-ket notation for this section. We write the initial one-particle wavefunction $|\varphi\rangle \in \mathfrak{h}$ in the computational basis: $|\varphi\rangle = \varphi_0|0\rangle + \varphi_1|1\rangle$. Let us choose $A^{(1)} = 0$ and $A^{(2)} = iZ \otimes Z$, where $Z = |0\rangle\langle 0| - |1\rangle\langle 1|$ is the third Pauli matrix. Similar anti-Hermitian interactions can be engineered in qubit systems [135]. We choose the following orthonormal basis of $\text{Sym}^N \mathbb{C}^2$, indexed by $n = 0, \dots, N$:

$$|N, n\rangle := \frac{1}{N!} \sqrt{\binom{N}{n}} \sum_{P \in S_N} P \left(|0\rangle^{\otimes n} \otimes |1\rangle^{\otimes (N-n)} \right), \quad (2.23)$$

where the sum runs over all the $N!$ permutations of N qubits. This basis diagonalizes the evolution operator:

$$-iA^{(N)}|N, n\rangle = \lambda_{N,n}|N, n\rangle, \quad \lambda_{N,n} = \frac{(N-2n)^2 - N}{2(N-1)}. \quad (2.24)$$

In this basis, the initial N -particle wavefunction has the form

$$|\Psi^{(N)}(0)\rangle = (\varphi_0|0\rangle + \varphi_1|1\rangle)^{\otimes N} = \sum_{n=0}^N \varphi_0^n \varphi_1^{N-n} \sqrt{\binom{N}{n}} |N, n\rangle, \quad (2.25)$$

and the solution of the evolution equation (2.2) becomes

$$|\Psi^{(N)}\rangle = \sum_{n=0}^N \varphi_0^n \varphi_1^{N-n} \sqrt{\binom{N}{n}} e^{\lambda_{N,n}t} |N, n\rangle. \quad (2.26)$$

To compute the unnormalized one-particle marginal state, we can compute the partial trace using the basis $\{|N-1, s\rangle\}_{s=0}^{N-1}$ of $\text{Sym}^{N-1}\mathbb{C}^2$:

$$\rho^{(1)} = \sum_{s=0}^{N-1} \langle N-1, s | \Psi^{(N)} \rangle \langle \Psi^{(N)} | N-1, s \rangle. \quad (2.27)$$

We have

$$\begin{aligned} & \langle N-1, s | N, n \rangle \\ &= \sum_{P \in S^N} \sum_{Q \in S^{N-1}} \frac{1}{N!(N-1)!} \sqrt{\binom{N}{n} \binom{N-1}{s}} Q \left(\langle 0 |^{\otimes s} \otimes \langle 1 |^{\otimes (N-1-s)} \right) P \left(|0\rangle^{\otimes n} \otimes |1\rangle^{\otimes (N-n)} \right) \\ &= \sum_{P \in S^N} \frac{1}{N!} \sqrt{\binom{N}{n} \binom{N-1}{s}} \left(\langle 0 |^{\otimes s} \otimes \langle 1 |^{\otimes (N-1-s)} \right) P \left(|0\rangle^{\otimes n} \otimes |1\rangle^{\otimes (N-n)} \right) \\ &= \frac{1}{N!} \sqrt{\binom{N}{n} \binom{N-1}{s}} n!(N-n)! \left(\delta_{n,s} |1\rangle + \delta_{n,s+1} |0\rangle \right) \\ &= \sqrt{\frac{\binom{N-1}{s}}{\binom{N}{n}}} (\delta_{n,s} |1\rangle + \delta_{n,s+1} |0\rangle). \end{aligned} \quad (2.28)$$

Plugging equation (2.26) in (2.27) and using (2.28) we obtain the matrix elements of

$\rho^{(1)}$:

$$\begin{aligned}
\rho_{00}^{(1)} &= |\varphi_0|^2 \sum_{s=0}^{N-1} |\varphi_1|^{2s} |\varphi_0|^{2(N-1-s)} \binom{N-1}{s} e^{2\lambda_{N,s}t}, \\
\rho_{01}^{(1)} &= \varphi_0 \varphi_1^* \sum_{s=0}^{N-1} |\varphi_0|^{2s} |\varphi_1|^{2(N-1-s)} \binom{N-1}{s} e^{(\lambda_{N,s+1} + \lambda_{N,s})t}, \\
\rho_{10}^{(1)} &= \varphi_1 \varphi_0^* \sum_{s=0}^{N-1} |\varphi_0|^{2s} |\varphi_1|^{2(N-1-s)} \binom{N-1}{s} e^{(\lambda_{N,s+1} + \lambda_{N,s})t}, \\
\rho_{11}^{(1)} &= |\varphi_1|^2 \sum_{s=0}^{N-1} |\varphi_0|^{2s} |\varphi_1|^{2(N-1-s)} \binom{N-1}{s} e^{2\lambda_{N,s}t}.
\end{aligned} \tag{2.29}$$

To analyze the evolution equation of the Hartree wavefunction (2.10), we write the wavefunction in the computational basis $|\phi\rangle = \phi_0|0\rangle + \phi_1|1\rangle$ with initial condition $|\phi(0)\rangle = |\varphi\rangle$ and get the equations

$$\begin{cases} \partial_t |\phi\rangle = (\langle\phi|Z|\phi\rangle Z - \langle\phi|Z|\phi\rangle^2) |\phi\rangle \\ |\phi(0)\rangle = |\varphi\rangle \end{cases} \Rightarrow \begin{cases} \partial_t \phi_0 = \left(|\phi_0|^2 - |\phi_1|^2 - (|\phi_0|^2 - |\phi_1|^2)^2 \right) \phi_0 \\ \partial_t \phi_1 = \left(|\phi_1|^2 - |\phi_0|^2 - (|\phi_0|^2 - |\phi_1|^2)^2 \right) \phi_1 \\ \phi_0(0) = \varphi_0, \quad \phi_1(0) = \varphi_1 \end{cases}. \tag{2.30}$$

The solution to these equations is

$$\phi_0 = e^{i\theta_0} \sqrt{\frac{1}{2} \left(1 + \frac{ke^{2t}}{\sqrt{1 + (ke^{2t})^2}} \right)}, \quad \phi_1 = e^{i\theta_1} \sqrt{\frac{1}{2} \left(1 - \frac{ke^{2t}}{\sqrt{1 + (ke^{2t})^2}} \right)}, \tag{2.31}$$

where

$$k := \frac{|\varphi_0|^2 - |\varphi_1|^2}{\sqrt{1 - (|\varphi_0|^2 - |\varphi_1|^2)^2}}, \quad \theta_i = \arg(\varphi_i). \tag{2.32}$$

Equation (2.30) has stable and unstable fixed points. Wavefunctions with $|\varphi_0|^2 = |\varphi_1|^2 = \frac{1}{2}$ are unstable fixed points, while the stable fixed points are given by $|\varphi\rangle = |0\rangle$ and $|\varphi\rangle = |1\rangle$.

We will show that the system can have the following three asymptotic behaviors for $N \rightarrow \infty$:

- Stable fixed points: if $|\varphi\rangle = |0\rangle$ or $|\varphi\rangle = |1\rangle$, the solution of the Hartree equation is constant in time and agrees with the one-particle marginal state for any N .
- Unstable fixed points after the critical time: if $|\varphi_0|^2 = |\varphi_1|^2 = \frac{1}{2}$, the solution of the Hartree equation is constant in time and agrees up to $t = \frac{1}{2}$ with the limit for

$N \rightarrow \infty$ of the one-particle marginal state. For $t > \frac{1}{2}$, such a limit becomes mixed, while the solution of the Hartree equation stays constant.

- Any other case: if $|\varphi_0| \neq |\varphi_1|$, the limit for $N \rightarrow \infty$ of the one-particle marginal state is pure but is different from the solution of the Hartree equation.

2.2.1 Large- N limit

In this section, we will compute the limit of the one-particle marginal state $\hat{\rho}^{(1)}$ for $N \rightarrow \infty$.

Let us first consider the initial conditions that are stable fixed points of the Hartree equation. We will consider only the case $|\varphi\rangle = |0\rangle$, since the case $|\varphi\rangle = |1\rangle$ is completely analogous. The solution to the N -body evolution equation (2.26) is $|\Psi^{(N)}\rangle = e^{\frac{Nt}{2}}|0\rangle^{\otimes N}$ and the one-particle marginal state is constant in time: $\hat{\rho}^{(1)} = |0\rangle\langle 0|$. The linear entropy and the infidelity with respect to the Hartree solution are $S_L = 0$, $I = 0$ and the Hartree approximation is exact at any time for any N .

In the remainder of this section, we will consider the initial conditions satisfying $|\varphi_0|^2, |\varphi_1|^2 \in (0, 1)$. We will use the Stirling's approximation of the factorial

$$\ln M! = M \ln M - M + \frac{1}{2} \ln(2\pi M) + \mathcal{O}(M^{-1}). \quad (2.33)$$

Then we can approximate the binomial distribution as

$$p^n q^{M-n} \binom{M}{n} \approx \exp \left(n \ln \frac{p(M-n)}{q n} + M \ln \frac{q M}{M-n} + \frac{1}{2} \ln \frac{M}{2\pi n(M-n)} \right). \quad (2.34)$$

We will use the substitution $s = Nx$ such that we can approximate the sum over s by an integral over x . We can also approximate the eigenvalues as

$$\lambda_{N,Nx} = \frac{N}{2}(1-2x)^2 - 2x(1-x) + \mathcal{O}(N^{-1}). \quad (2.35)$$

We rewrite $\rho_{00}^{(1)}$ as

$$\rho_{00}^{(1)} = \sum_{s=0}^N |\varphi_1|^{2s} |\varphi_0|^{2(N-s)} \frac{N-s}{N} \binom{N}{s} e^{2\lambda_{N,s}t}. \quad (2.36)$$

Applying the Stirling's approximation (2.34), replacing $s = Nx$, using (2.35) and approximating the sum by an integral, we get the following expression:

$$\rho_{00}^{(1)} \approx \sqrt{\frac{N}{2\pi}} \int_0^1 dx \sqrt{\frac{1-x}{x}} e^{Nf_t(x) - 4tx(1-x)}, \quad (2.37)$$

where

$$f_t(x) = x \ln \frac{|\varphi_1|^2(1-x)}{|\varphi_0|^2 x} + \ln \frac{|\varphi_0|^2}{1-x} + t(1-2x)^2, \quad (2.38)$$

and its derivatives are

$$f'_t(x) = \ln \frac{|\varphi_1|^2}{|\varphi_0|^2} + \ln \frac{1-x}{x} - 4t(1-2x), \quad (2.39)$$

$$f''_t(x) = 8t - \frac{1}{x(1-x)}. \quad (2.40)$$

The integral (2.37) can be further approximated using the Laplace's method [136, 137]. In the limit of large N , the major contributions to the integral come from the values of x near the global maximizers of f_t . In the neighborhood of these points, we can approximate the integrand by a Gaussian function using a Taylor expansion for f_t . Since the tails of these integrands decay exponentially, we can extend the integral to the whole real line. In this way, we can integrate analytically the Gaussian function. Let $\{x_i\}$ be the global maximizers of f_t . Recall that $|\varphi_0|^2, |\varphi_1|^2 \in (0, 1)$. The derivative (2.39) satisfies $\lim_{x \rightarrow 0+} f'_t(x) = +\infty$ and $\lim_{x \rightarrow 1-} f'_t(x) = -\infty$. Then, all the global maximizers of f_t lie in $(0, 1)$ and satisfy $f'_t(x_i) = 0$, $f''_t(x_i) \leq 0$. The Laplace's method applied to equation (2.37) gives

$$\rho_{00}^{(1)} \approx \sum_i \sqrt{\frac{N}{2\pi}} \sqrt{\frac{1-x_i}{x_i}} e^{Nf_t(x_i) - 4tx_i(1-x_i)} \int_{-\infty}^{\infty} dx e^{\frac{N}{2}f''_t(x_i)(x-x_i)^2}. \quad (2.41)$$

Using the Gaussian integral $\int_{-\infty}^{\infty} e^{-y^2} dy = \sqrt{\pi}$, the result is

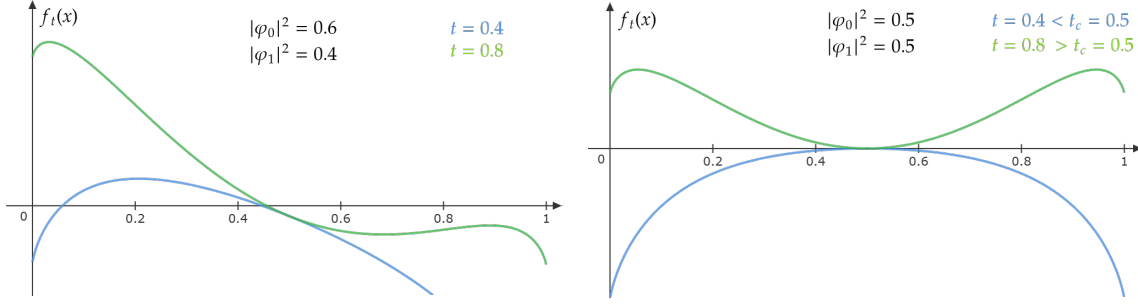
$$\rho_{00}^{(1)} \approx \sum_i \sqrt{\frac{1}{-f''_t(x_i)}} \sqrt{\frac{1-x_i}{x_i}} e^{Nf_t(x_i) - 4tx_i(1-x_i)}. \quad (2.42)$$

We will show that for any initial condition with $|\varphi_0|^2 \neq |\varphi_1|^2$, f_t has a single global maximizer. In Figure 2.1a, we plot the function f_t for a generic initial condition. f_t may have one or two local maximizers, but only one of them is a global maximizer. Only for the exceptional initial condition $|\varphi_0|^2 = |\varphi_1|^2 = \frac{1}{2}$ and $t > \frac{1}{2}$ there are two global maximizers (see Figure 2.1b).

To prove the uniqueness of the global maximizer, we start by analyzing the function $f''_t(x)$ given by equation (2.40). At times $t < \frac{1}{2}$, the second derivative is always negative: $f''_t(x) < 0 \forall x \in (0, 1)$. Hence f'_t is strictly decreasing and f_t has a single local maximizer, which is then the unique global maximizer. At times $t > \frac{1}{2}$, since equation (2.40) is symmetric with respect to $x = \frac{1}{2}$, f''_t has two symmetric roots

$$r_{\pm} = \frac{1}{2} \left(1 \pm \sqrt{1 - \frac{1}{2t}} \right), \quad (2.43)$$

which split the interval $(0, 1)$ into three sub-intervals. f''_t is positive in the central sub-interval and negative in the other two. When f_t has two local maximizers, one of them is



(a) For initial conditions satisfying $|\varphi_0|^2 \neq |\varphi_1|^2$, the function f_t can have one or two local maximizers, but it always has a single global maximizer.

(b) For the initial conditions satisfying $|\varphi_0|^2 = |\varphi_1|^2 = \frac{1}{2}$, the function f_t has a single local maximizer $x = \frac{1}{2}$ for $t \leq \frac{1}{2}$ and it has two symmetric global maximizers for $t > \frac{1}{2}$.

Figure 2.1: Plot of f_t as a function of x , as defined in (2.38), for different instances of initial condition and time.

larger than r_+ and the other one is smaller than r_- . To determine which one is a global maximizer, we observe that if x_t^* is a global maximizer then

$$f_t(x_t^*) \geq f_t(1 - x_t^*) = f_t(x_t^*) + (1 - 2x_t^*) \ln \frac{|\varphi_1|^2}{|\varphi_0|^2}, \quad (2.44)$$

and

$$(1 - 2x_t^*) \ln \frac{|\varphi_1|^2}{|\varphi_0|^2} \leq 0. \quad (2.45)$$

If $|\varphi_0|^2 > |\varphi_1|^2$, the unique global maximizer satisfies $x_t^* < r_-$. If $|\varphi_0|^2 < |\varphi_1|^2$, the unique global maximizer satisfies $x_t^* > r_+$. If $|\varphi_0|^2 = |\varphi_1|^2 = \frac{1}{2}$, the equation (2.45) is trivially satisfied and there are two global maximizers which are symmetric with respect to $\frac{1}{2}$.

One can compute the evolution equation of the global maximizer implicitly using $f_t'(x_t^*) = 0$:

$$\partial_t x_t^* = \frac{4(1 - 2x_t^*)}{8t - \frac{1}{x_t^*(1 - x_t^*)}}. \quad (2.46)$$

At time $t < \frac{1}{2}$ the denominator is strictly negative. At time $t > \frac{1}{2}$ the denominator vanishes if the equation (2.40) vanishes. If a point satisfies $f_t'(x) = 0$ and $f_t''(x) = 0$, then it is a saddle point and it is not the global maximizer, unless $f_t'''(x) = 0$, which only happens at $x = \frac{1}{2} \in (r_-, r_+)$. Then, the denominator of (2.46) never vanishes, and the trajectory of the global maximizer is continuous.

At the critical time $t_c = \frac{1}{2}$, the trajectory can be discontinuous only if the maximizer is $x_{\frac{1}{2}}^* = \frac{1}{2}$ and this happens only in the exceptional case $|\varphi_0|^2 = |\varphi_1|^2$. In this case, $x_t^* = \frac{1}{2}$ at $t \leq \frac{1}{2}$ and at later times there are two global maximizers.

Single global maximizer

For the initial conditions such that $|\varphi_0|^2 \neq |\varphi_1|^2$ or $|\varphi_0|^2 = |\varphi_1|^2$ and $t \leq \frac{1}{2}$, we showed that there is a unique global maximizer x_t^* . Equation (2.42) becomes

$$\rho_{00}^{(1)} \approx \frac{1}{\sqrt{-f_t''(x_t^*)}} \sqrt{\frac{1-x_t^*}{x_t^*}} \exp \left(N f_t(x_t^*) - 4t x_t^* (1-x_t^*) \right). \quad (2.47)$$

A similar computation allows us to compute the remaining matrix elements:

$$\rho_{11}^{(1)} \approx \frac{1}{\sqrt{-f_t''(x_t^*)}} \sqrt{\frac{x_t^*}{1-x_t^*}} \exp \left(N f_t(x_t^*) - 4t x_t^* (1-x_t^*) \right), \quad (2.48)$$

$$\rho_{10}^{(1)} = \rho_{01}^{(1)*} \approx \frac{\varphi_0^*}{\varphi_1^*} \frac{1}{\sqrt{-f_t''(x_t^*)}} \sqrt{\frac{x_t^*}{1-x_t^*}} \exp \left(N f_t(x_t^*) - 4t x_t^* (1-x_t^*) + 2t(1-2x_t^*) \right). \quad (2.49)$$

When normalizing the state, all the N dependence cancels and we get the limit of the one-particle marginal state for the case where f_t has a single global maximizer:

$$\lim_{N \rightarrow \infty} \hat{\rho}^{(1)} = \begin{pmatrix} 1-x_t^* & e^{i\theta} \sqrt{x_t^*(1-x_t^*)} \\ e^{-i\theta} \sqrt{x_t^*(1-x_t^*)} & x_t^* \end{pmatrix}, \quad (2.50)$$

where $e^{-i\theta} = \frac{\varphi_0^*}{|\varphi_0|} \frac{|\varphi_1|}{\varphi_1^*}$. Observe that the limit state (2.50) is pure and can be characterized by a one-particle wavefunction: $\lim_{N \rightarrow \infty} \hat{\rho}^{(1)} =: |\nu\rangle\langle\nu|$, where $|\nu\rangle = \nu_0|0\rangle + \nu_1|1\rangle$ defined up to a global phase by

$$\nu_0 = e^{i\theta} \sqrt{1-x_t^*}, \quad \nu_1 = \sqrt{x_t^*}. \quad (2.51)$$

In order to compare it with the Hartree evolution, we derive the evolution equation for $|\nu\rangle$ using the implicit time evolution equation (2.46) for the global maximizer and we write it in terms of its components using equation (2.51). The evolution equation for the one-particle wavefunction $|\nu\rangle$ is

$$\begin{cases} \partial_t \nu_0 = \frac{|\nu_0|^2 - |\nu_1|^2 - (|\nu_0|^2 - |\nu_1|^2)^2}{1 - 8t|\nu_0|^2|\nu_1|^2} \nu_0 \\ \partial_t \nu_1 = \frac{|\nu_1|^2 - |\nu_0|^2 - (|\nu_0|^2 - |\nu_1|^2)^2}{1 - 8t|\nu_0|^2|\nu_1|^2} \nu_1, \end{cases} \quad (2.52)$$

and matches the Hartree equation (2.30) only at $t = 0$ or at the fixed points. This is a counterexample to the generalization of the mean-field theory to non-Hermitian Hamiltonians.

Double global maximizer

For initial conditions such that $|\varphi_0|^2 = |\varphi_1|^2 = \frac{1}{2}$, for $t > \frac{1}{2}$ f_t has two symmetric global maximizers $x_t^* \in (0, \frac{1}{2})$ and $1 - x_t^* \in (\frac{1}{2}, 1)$. Evaluating the approximation (2.42) we obtain

$$\rho_{00}^{(1)} \approx \frac{1}{\sqrt{-f_t''(x_t^*)}} \left(\sqrt{\frac{1-x_t^*}{x_t^*}} + \sqrt{\frac{x_t^*}{1-x_t^*}} \right) \exp \left(N f_t(x_t^*) - 4t x_t^* (1-x_t^*) \right). \quad (2.53)$$

By symmetry we know that $\rho_{11}^{(1)} = \rho_{00}^{(1)}$. Using the same methods we can compute the non diagonal terms

$$\rho_{01}^{(1)} = \rho_{10}^{(1)*} \approx \frac{2e^{i\theta}}{\sqrt{-f_t''(x_t^*)}} \exp \left(N f_t(x_t^*) - 4t x_t^* (1-x_t^*) \right). \quad (2.54)$$

Normalizing by the trace we get the limit of the one-particle marginal state in the case of two global maximizers:

$$\lim_{N \rightarrow \infty} \hat{\rho}^{(1)} = \begin{pmatrix} e^{-i\theta} \sqrt{\frac{1}{x_t^*(1-x_t^*)}} & e^{i\theta} \sqrt{\frac{x_t^*(1-x_t^*)}{\frac{1}{2}}} \\ e^{-i\theta} \sqrt{\frac{x_t^*(1-x_t^*)}{\frac{1}{2}}} & e^{i\theta} \sqrt{\frac{1}{x_t^*(1-x_t^*)}} \end{pmatrix}. \quad (2.55)$$

The linear entropy of this matrix is

$$S_L \left(\lim_{N \rightarrow \infty} \hat{\rho}^{(1)} \right) = \frac{1}{2} - 2x_t^*(1-x_t^*) > 0, \quad (2.56)$$

hence the limiting state is mixed and cannot be described by the solution of the Hartree equation. Furthermore, in the limit $t \rightarrow \infty$ we have $0 < x_t^* < r_- \rightarrow 0$, and the limiting one-particle state tends to the maximally mixed state for $t \rightarrow \infty$. We also notice that the limit for $N \rightarrow \infty$ of the one-particle marginal state (2.55) can be written as the mixture of two pure states that come from the contribution of the two maximizers of f_t .

2.2.2 Numerical analysis

In the previous section, we have analytically computed the one-particle marginal state in the limit of infinitely many particles. We have found that for almost every initial condition, such limit is pure but does not satisfy the non-Hermitian Hartree equation. For the exceptional initial conditions $|\varphi_0|^2 = |\varphi_1|^2 = \frac{1}{2}$, there is a critical time after which the limiting state becomes mixed. In this section, we will compare the solution of the non-Hermitian Hartree equation (2.31) with the one-particle marginal state for finite N (2.29).

Linear entropy of the one-particle marginal state

In Figure 2.2, we plot the linear entropy (2.11) of the one-particle marginal state (2.29):

- In Figure 2.2a, we show that for initial conditions such that $|\varphi_0|^2 \neq |\varphi_1|^2$, the linear entropy tends to zero for $N \rightarrow \infty$.
- In Figure 2.2b, we show that for initial conditions such that $|\varphi_0|^2 = |\varphi_1|^2 = \frac{1}{2}$, for $N \rightarrow \infty$ the linear entropy tends to zero up to $t = \frac{1}{2}$, but has a nonzero limit for $t > \frac{1}{2}$.
- In Figure 2.2c, we show that the linear entropy scales as $\mathcal{O}(N^{-1})$ for $N \rightarrow \infty$ for initial conditions such that $|\varphi_0|^2 \neq |\varphi_1|^2$.
- In Figure 2.2d, we show that the linear entropy still scales as $\mathcal{O}(N^{-1})$ for $N \rightarrow \infty$ for initial conditions such that $|\varphi_0|^2 = |\varphi_1|^2 = \frac{1}{2}$ for $t < \frac{1}{2}$.

Infidelity with respect to the solution of the Hartree equation

In Figure 2.3, we analyze the infidelity (2.12) of the one-particle marginal state with respect to the solution of the Hartree equation:

- In Figure 2.3a, we show that for initial conditions such that $|\varphi_0|^2 \neq |\varphi_1|^2$, the infidelity has a nonzero limit for $N \rightarrow \infty$, and therefore the Hartree equation does not describe the time evolution of the one-particle marginal state.
- In Figure 2.3b, we show that for initial conditions such that $|\varphi_0|^2 = |\varphi_1|^2 = \frac{1}{2}$, the infidelity tends to zero for $N \rightarrow \infty$ up to $t = \frac{1}{2}$, but has a nonzero limit for $t > \frac{1}{2}$. Therefore, the Hartree equation correctly describes the time evolution of the one-particle marginal state only up to $t = \frac{1}{2}$.

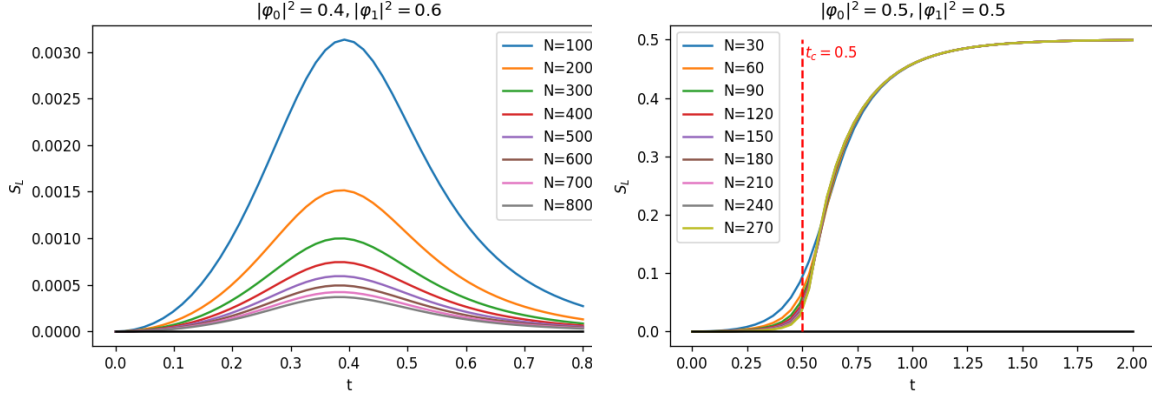
Convergence speed towards the limit for $N \rightarrow \infty$

The last numerical analysis concerns the speed of the convergence of the one-particle marginal state towards its limit for $N \rightarrow \infty$. We define the infidelity of the one-particle marginal state $\hat{\rho}^{(1)}$ with respect to its limit for $N \rightarrow \infty$ as

$$\varepsilon = 1 - F\left(\hat{\rho}^{(1)}, \lim_{N \rightarrow \infty} \hat{\rho}^{(1)}\right), \quad (2.57)$$

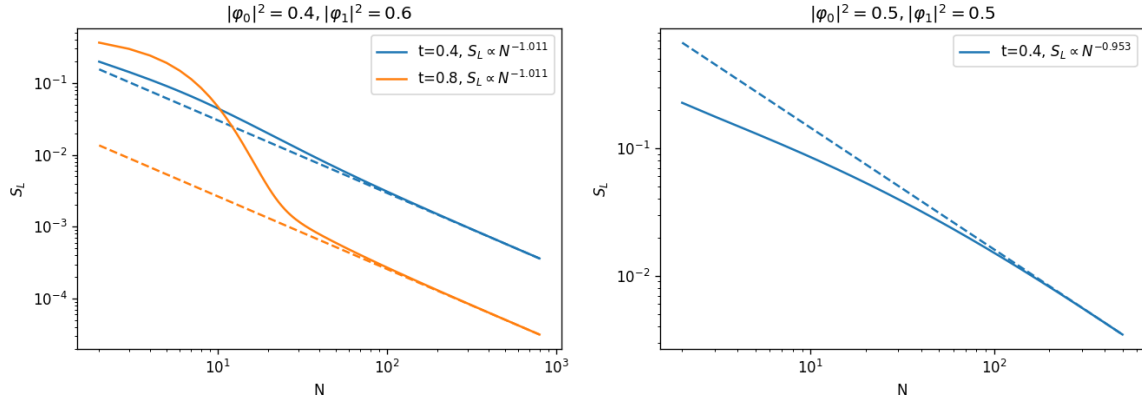
where the fidelity between the quantum states ρ and σ is

$$F(\rho, \sigma) = \left(\text{Tr} \sqrt{\sqrt{\rho} \sigma \sqrt{\rho}} \right)^2 \quad (2.58)$$



(a) Initial conditions with $|\varphi_0|^2 \neq |\varphi_1|^2$. Time is plotted in the horizontal axis. At any time, the linear entropy tends to zero for $N \rightarrow \infty$.

(b) Initial conditions with $|\varphi_0|^2 = |\varphi_1|^2 = \frac{1}{2}$. Time is plotted in the horizontal axis. For $t > \frac{1}{2}$, the linear entropy has a nonzero limit for $N \rightarrow \infty$.



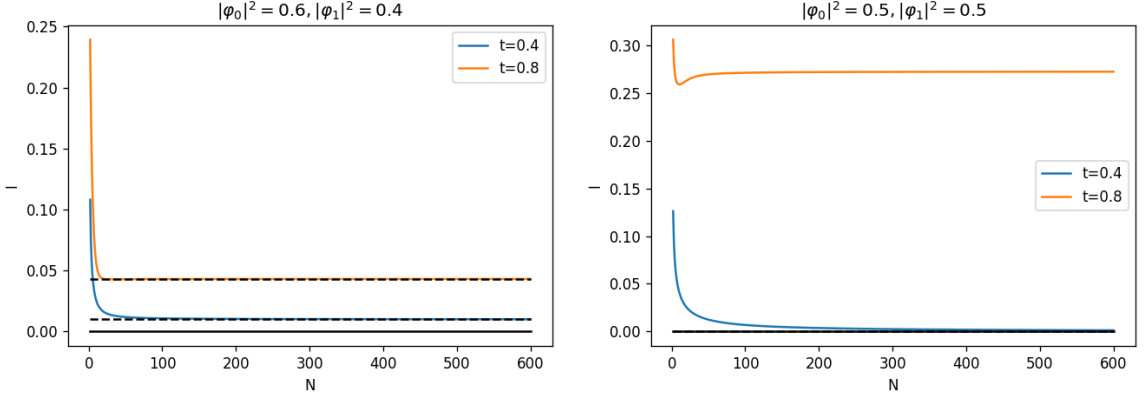
(c) N is plotted in the horizontal axis. The linear entropy scales as $\mathcal{O}(N^{-1})$ at every time.

(d) N is plotted in the horizontal axis. The linear entropy scales as $\mathcal{O}(N^{-1})$ for $t < \frac{1}{2}$.

Figure 2.2: Linear entropy of the one-particle marginal states of the solution of the N -particle equation. Solid lines show the numerical computation of the linear entropy. We fit the tails of the curves (last 20%) with the function aN^b . The fit is plotted in dashed lines and the values of the exponents b are written in the legends.

and the value of x_t^* is found by numerically minimizing $f_t(x)$.

In Figure 2.4a, we show that the infidelity always tends to zero for $N \rightarrow \infty$ (as it should). In Figure 2.4b, we show that the infidelity scales as $\mathcal{O}(N^{-1})$ for $N \rightarrow \infty$ both for initial conditions such that $|\varphi_0|^2 \neq |\varphi_1|^2$ and for initial conditions such that $|\varphi_0|^2 = |\varphi_1|^2 = \frac{1}{2}$ and $t < \frac{1}{2}$, matching the scaling in the Hermitian case. Instead, for initial conditions such



(a) For initial conditions such that $|\varphi_0|^2 \neq |\varphi_1|^2$, the infidelity has a nonzero limit for $N \rightarrow \infty$, and the Hartree equation does not describe the time evolution of the one-particle marginal state.

(b) For initial conditions such that $|\varphi_0|^2 = |\varphi_1|^2 = \frac{1}{2}$, the infidelity tends to zero for $N \rightarrow \infty$ for $t < \frac{1}{2}$, but has a nonzero limit for $t > \frac{1}{2}$. Therefore, the Hartree equation describes the time evolution of the one-particle marginal state only up to $t = \frac{1}{2}$.

Figure 2.3: Numerical computation of the infidelity of the one-particle marginal state with respect to the solution of the Hartree equation. Dashed lines corresponds to the limit of the infidelity for $N \rightarrow \infty$ using the results of section 2.2.1.

that $|\varphi_0|^2 = |\varphi_1|^2 = \frac{1}{2}$ and $t > \frac{1}{2}$, the infidelity scales as $\mathcal{O}(N^{-2})$.

2.2.3 Analysis of the second time derivative

In this subsection, we use the equation (2.22) for the second time derivative of the difference between the one-particle reduced density matrix and the Hartree solution and we will show that this equation can tell us the initial conditions for which the approximation works.

In the present example, equation (2.22) can be written in the form

$$\lim_{N \rightarrow \infty} \partial_t^2 (\hat{\rho}^{(1)} - \gamma)|_{t=0} = 2\langle \varphi | Z | \varphi \rangle (1 - \langle \varphi | Z | \varphi \rangle^2) (Z - \langle \varphi | Z | \varphi \rangle) |\varphi \rangle \langle \varphi| + h.c. . \quad (2.59)$$

There are only two types of initial conditions for which this equation vanishes. One can see that the term $\langle \varphi | Z | \varphi \rangle$ vanishes for the exceptional points $|\varphi_0| = |\varphi_1|$ and the term $(1 - \langle \varphi | Z | \varphi \rangle^2)$ vanishes for the eigenvectors of the Z operator: $|\varphi_0| = 0, |\varphi_1| = 1$ and $|\varphi_0| = 1, |\varphi_1| = 0$. Also, the vector equation $(Z - \langle \varphi | Z | \varphi \rangle) |\varphi \rangle = 0$ vanishes only in the eigenvector of the Z operator.

The condition $\partial_t^2 (\hat{\rho}^{(1)} - \gamma)|_{t=0} = \mathcal{O}(N^{-1})$ is a necessary condition for the success of the Hartree approximation. However, in this example, it gives us the only initial conditions for which the approximation works. In the case of the eigenvalues of the Z operators, the

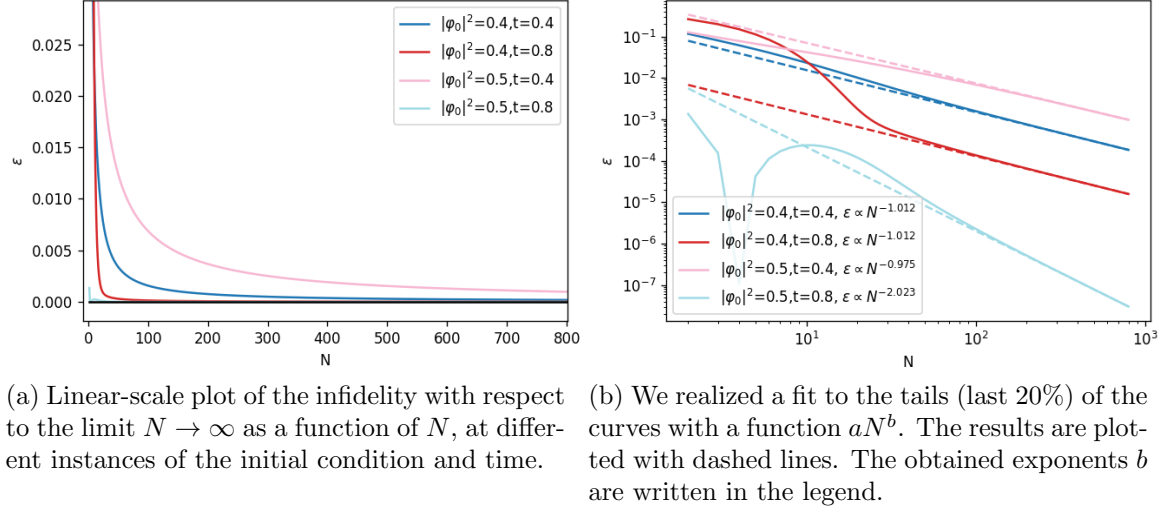


Figure 2.4: Numerical computation of the infidelity of the one-particle marginal state with respect to its limit for $N \rightarrow \infty$. The infidelity scales as $\mathcal{O}(N^{-1})$ for $N \rightarrow \infty$ for almost all initial conditions, and scales as $\mathcal{O}(N^{-2})$ for the initial conditions such that $|\varphi_0|^2 = |\varphi_1|^2 = \frac{1}{2}$ and $t > \frac{1}{2}$.

initial state is a stable fixed point of the Hartree equation and the many body state is an eigenvalue of the many body Hamiltonian, then the evolution is trivial in both cases and the approximation is exact. In the case of the exceptional points, the initial state is an instable fixed point of the Hartree equation and despite the non-trivial evolution of the many body equation, the one-particle reduced density matrix is time independent up to the critical time, in this time interval the approximation works.

2.3 Non-Hermitian ZZ interaction with real spectrum

As a counterexample to the mean-field approximation, we considered in section 2.2 a purely anti-Hermitian Hamiltonian. Since its eigenvalues are purely imaginary, the dynamics of the normalized wavefunction converges exponentially fast to the eigenvectors with maximum eigenvalues. The same effect would take place for a generic purely anti-Hermitian Hamiltonian: the wavefunction would converge exponentially fast to the eigenvector associated to the eigenvalue with largest imaginary part. In order to avoid this effect, we construct an example of a non-Hermitian Hamiltonian with real spectrum.

As in the previous example, we take $\mathfrak{h} = \mathbb{C}^2$, the qubit Hilbert space, choose a non-orthogonal basis of $\mathfrak{h}$ given by normalized vectors $\{|v_0\rangle, |v_1\rangle\}$, and define the change of

basis given by the operator

$$C := |v_0\rangle\langle 0| + |v_1\rangle\langle 1|. \quad (2.60)$$

Let us consider the interaction between two particles given by $A^{(2)} = CZC^{-1} \otimes CZC^{-1}$. The corresponding mean-field Hamiltonian for N particles is given by

$$A^{(N)} = \frac{1}{N-1} \sum_{1 \leq i < j \leq N} (CZC^{-1})_i (CZC^{-1})_j. \quad (2.61)$$

In order to diagonalize it, we rewrite it as

$$A^{(N)} = C^{\otimes N} \frac{1}{2(N-1)} \left(\left(\sum_{i=1}^N Z_i \right)^2 - N \right) (C^{-1})^{\otimes N}. \quad (2.62)$$

Similarly to (2.24), the eigenvalues and eigenvectors of $A^{(N)}$ are given by

$$A^{(N)} C^{\otimes N} |N, n\rangle = \lambda_{N,n} C^{\otimes N} |N, n\rangle, \quad \lambda_{N,n} = \frac{(N-2n)^2 - N}{2(N-1)}. \quad (2.63)$$

Observe that the spectrum is real. We quantify the non-Hermiticity induced by the change of basis C with the overlap $\alpha = \langle v_0 | v_1 \rangle$. Then we can compute

$$C^\dagger C = \mathbb{I} + \alpha |v_0\rangle\langle v_1| + \alpha^* |v_1\rangle\langle v_0|. \quad (2.64)$$

Even if the spectrum is real, since the Hamiltonian is not Hermitian, the eigenvectors of $A^{(N)}$ are not orthogonal, instead they satisfy

$$\langle N, n | C^{\dagger \otimes N} C^{\otimes N} |N, m\rangle = \frac{1}{\sqrt{\binom{N}{m} \binom{N}{n}}} \sum_a \alpha^{n-a} \alpha^{*m-a} \binom{N}{a, n-a, m-a, N-m-n+a}. \quad (2.65)$$

Before solving the Schrödinger equation (2.2) with initial state $|\Psi^{(N)}(0)\rangle = |\varphi\rangle^{\otimes N}$, we need to write the initial state in the eigenbasis. Let us define $|\eta\rangle = \eta_0|0\rangle + \eta_1|1\rangle := C^{-1}|\varphi\rangle$, which is not normalized if C is not unitary. So the initial state is given by $|\Psi^{(N)}(0)\rangle = (C|\eta\rangle)^{\otimes N}$. Then the decomposition of the initial state in the eigenbasis of the non-Hermitian Hamiltonian is given by

$$|\Psi^{(N)}(0)\rangle = \sum_{n=0}^N \eta_0^n \eta_1^{N-n} \sqrt{\binom{N}{n}} C^{\otimes N} |N, n\rangle, \quad (2.66)$$

the time evolution is given by

$$|\Psi^{(N)}(t)\rangle = \sum_{n=0}^N \eta_0^n \eta_1^{N-n} \sqrt{\binom{N}{n}} e^{-i\lambda_{N,n}t} C^{\otimes N} |N, n\rangle, \quad (2.67)$$

and the one-particle reduced density matrix is given by

$$\rho^{(1)} = \sum_{m,n=0}^N \eta_0^n \eta_1^{N-n} \eta_0^{*m} \eta_1^{*N-m} \sqrt{\binom{N}{n} \binom{N}{m}} e^{-i(\lambda_{N,n} - \lambda_{N,m})t} \text{Tr}_{2\dots N} (C^{\otimes N} |N, n\rangle \langle N, m| C^{\dagger \otimes N}). \quad (2.68)$$

Using the non-orthogonality (2.65), we can write the exact evolution of the reduced density matrix in the chosen basis:

$$\begin{aligned} \rho^{(1)} = & \sum_{\substack{n_0, n_1, n_2, n_3 \geq 0 \\ \sum n_l = N-1}} |\eta_0|^{2n_0} |\eta_1|^{2n_1} (\eta_0 \eta_1^* \alpha^*)^{n_2} (\eta_0^* \eta_1 \alpha)^{n_3} \binom{N-1}{n_0, n_1, n_2, n_3} \\ & \times \left(\sum_{i,j=0}^1 e^{-it(\lambda_{N,n_2+n_0+1-i} - \lambda_{N,n_3+n_0+1-j})} \eta_i |v_i\rangle \langle v_j| \eta_j^* \right). \end{aligned} \quad (2.69)$$

We are going to compare the exact normalized single-particle evolution with the non-Hermitian Hartree equation (2.10). In this example, it takes the form

$$i\partial_t |\phi\rangle = \langle \phi | C Z C^{-1} | \phi \rangle C Z C^{-1} | \phi \rangle - i \text{Im} (\langle \phi | C Z C^{-1} | \phi \rangle^2) | \phi \rangle. \quad (2.70)$$

2.3.1 Hermitian case

We start by analyzing the Hermitian case in order to understand how the reduced density matrix actually converges to the solution of the Hartree equation. Set $\alpha = 0$ in (2.69) to compute the reduced density matrix. Using that $\alpha^n = \delta_{n,0}$, and the binomial theorem, the reduced density matrix simplifies to:

$$\begin{aligned} \rho^{(1)} = & |\eta_0|^2 |v_0\rangle \langle v_0| + \eta_0 \eta_1^* \left(|\eta_0|^2 e^{-i\frac{2t}{N-1}} + |\eta_1|^2 e^{i\frac{2t}{N-1}} \right)^{N-1} |v_0\rangle \langle v_1| \\ & + \eta_0^* \eta_1 \left(|\eta_0|^2 e^{i\frac{2t}{N-1}} + |\eta_1|^2 e^{-i\frac{2t}{N-1}} \right)^{N-1} |v_1\rangle \langle v_0| + |\eta_1|^2 |v_1\rangle \langle v_1|. \end{aligned} \quad (2.71)$$

A straightforward calculation of the linear entropy, defined in (2.11), gives

$$S_L(\rho^{(1)}) = 2|\eta_0|^2 |\eta_1|^2 \left(1 - \left[1 + 2|\eta_0|^2 |\eta_1|^2 \left(\cos \left(\frac{4t}{N-1} \right) - 1 \right) \right]^{(N-1)} \right). \quad (2.72)$$

We argued that the mean-field approximation requires that $\lim_{N \rightarrow \infty} S_L(\rho^{(1)}) = 0$ at any fixed time and indeed, it is true for (2.72). If we expand it for large N we obtain

$$S_L(\rho^{(1)}) = \frac{(8|\eta_0|^2 |\eta_1|^2 t)^2}{N} + \mathcal{O} \left(\frac{1}{N^2} \right). \quad (2.73)$$

But we make the observation that for any fixed number of particles, the linear entropy is a periodic function of time with period $(N - 1)/8\pi$ and it has the maximum value

$$\max_t S_L(\rho^{(1)}) = 2|\eta_0|^2|\eta_1|^2 \left(1 - (1 - 4|\eta_0|^2|\eta_1|^2)^{N-1}\right). \quad (2.74)$$

This value increases with N and tends to $2|\eta_0|^2|\eta_1|^2$ for $N \rightarrow \infty$. So the maximum possible value of the linear entropy over time increases with the number of particles, but the time required to achieve this value increases linearly in the number of particles, in such a way that when time is fixed we have the convergence towards a pure state following (2.73).

Since the one-particle reduced density matrix converges to a pure state, we can compare it with the solution of the Hartree equation (2.70). Since $\alpha = 0$, then $C^{-1} = C^\dagger$, then the Hartree equation takes the form

$$i\partial_t|\phi\rangle = \langle\phi, C Z C^\dagger\phi\rangle C Z C^\dagger|\phi\rangle, \quad (2.75)$$

with initial value $|\phi(0)\rangle = C|\eta\rangle$. Given that $z_0 = \langle\phi, C Z C^\dagger\phi\rangle$ is a constant of motion, the solution to (2.75) is $|\phi\rangle = C e^{-iz_0 Z t}|\eta\rangle$. We can then compute the infidelity (2.12) between the exact one-particle reduced density matrix and the Hartree approximation and we get

$$I = 2|\eta_0|^2|\eta_1|^2 \left(1 - \operatorname{Re} \left(\left(|\eta_0|^2 e^{i\frac{1-z_0}{N-1}t} + |\eta_1|^2 e^{-i\frac{1+z_0}{N-1}t} \right)^{N-1} \right) \right). \quad (2.76)$$

Similarly to the linear entropy (2.72), the infidelity is also a periodic function of time, with period that grows linearly with the number of particles and at fixed time it converges to zero for $N \rightarrow \infty$:

$$I = \frac{16|\eta_0|^4|\eta_1|^4 t^2}{N} + \mathcal{O}\left(\frac{1}{N^2}\right). \quad (2.77)$$

This shows, as it is known for all Hermitian Hamiltonians, that the Hartree equation correctly reproduces the one-particle reduced density matrix for any fixed time in the limit $N \rightarrow \infty$.

2.3.2 Numerical analysis of the non-Hermitian case

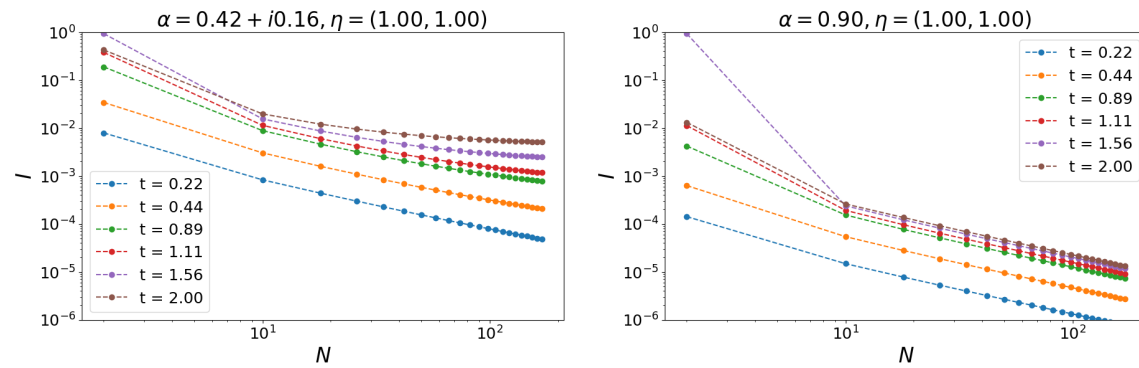
When $\alpha \neq 0$, the Hartree equation (2.70) is not solvable analytically, and the sum in (2.69) cannot be simplified using the binomial theorem. So we proceed with the numerical computation of these quantities.

The Hartree equation can easily be integrated numerically with standard methods, in particular we use the explicit Runge-Kutta method of order 5 implemented in the library Scipy in Python. The numerical computation of (2.69) is not stable since there might be very large numbers coming from the multinomial coefficient $\binom{N-1}{n_0, n_1, n_2, n_3} = \tilde{\mathcal{O}}(4^N)$, with different phases, coming from $(\eta_0 \eta_1^* \alpha^*)^{n_2} (\eta_0^* \eta_1 \alpha)^{n_3}$. Computing such differences between large numbers requires a float precision that scales linearly with N . This approach is very

expensive computationally and it does not allow to reach large values of N . In order to avoid this large cancellations problem, we restrict the initial data such that $\text{Re}(\alpha\eta_0^*\eta_1) > 0$. We observed numerically that in these cases the numerical instabilities were not a problem so we can compute $\rho^{(1)}$ using 64-bit floats.

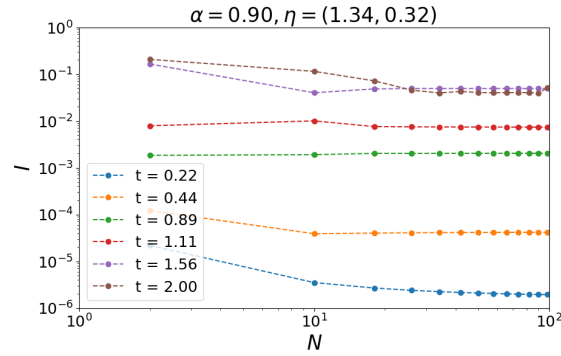
By computing several instances satisfying $\text{Re}(\alpha\eta_0^*\eta_1) > 0$, we observe that the infidelity does not always vanish for large N , showing that even if the eigenvalues of the Hamiltonian are real, non-Hermiticity can break the mean-field approximation. To depict the possible behaviors of the system as a function of the number of particles, we plot in Figure 2.5 the infidelity defined in (2.12) for three different instances.

In Figure 2.5b, where $\alpha > 0$ and $\eta_0 = \eta_1$, the infidelity vanishes, showing that the



(a) The infidelity converges to a non-zero value.

(b) The infidelity vanishes at large N .



(c) The infidelity converges very quickly to a non-zero value.

Figure 2.5: We numerically compute the infidelity (2.12) between the reduced density matrix (2.69) and the solution of the Hartree equation (2.70). We plot I as a function of the number of particles N in log-log scale for fixed times, and for three different choices of α and η . Observe that Figure 2.5a and Figure 2.5b have the same η , and Figure 2.5b and Figure 2.5c have the same α . The infidelity converges to zero only in Figure 2.5b.

approximation holds for this particular case. However, if we change either α (Figure 2.5a) or η (Figure 2.5c), the approximation breaks and the infidelity converges to some nonzero value.

2.3.3 Analysis of the second time derivative

We are going to use the equation (2.22) to analyze the set of initial conditions η and non-Hermiticity α such that the Hartree equation describes correctly the second time derivative. In order to simplify the notation we define $\mathcal{Z} = CZC^{-1}$. In this example, equation (2.22) reads

$$\begin{aligned} \partial_t^2(\hat{\rho}^{(1)} - \gamma)|_{t=0} = & \left(-\langle \varphi | \mathcal{Z} | \varphi \rangle + \langle \varphi | \mathcal{Z}^\dagger \mathcal{Z} | \varphi \rangle + \langle \varphi | \mathcal{Z} | \varphi \rangle^3 - \langle \varphi | \mathcal{Z}^\dagger | \varphi \rangle^2 \langle \varphi | \mathcal{Z} | \varphi \rangle \right) (\mathcal{Z} - \langle \varphi | \mathcal{Z} | \varphi \rangle) | \varphi \rangle \langle \varphi | + h.c. \\ & + \mathcal{O}(N^{-1}). \end{aligned} \quad (2.78)$$

A necessary condition for the Hartree approximation to describe the system is that this equation must vanish at the first order. This happens if one of the two terms in parenthesis vanishes, let's analyze each case separately.

The first case is given by the condition

$$(\mathcal{Z} - \langle \varphi | \mathcal{Z} | \varphi \rangle) | \varphi \rangle = 0. \quad (2.79)$$

This equation implies that the initial condition φ is an eigenvector of the operator $\mathcal{Z}$. In this case, the evolution of the Hartree solution and of the many-body equation is trivial and then the Hartree approximation is exact.

The second case is given by the condition

$$-\langle \varphi | \mathcal{Z} | \varphi \rangle + \langle \varphi | \mathcal{Z}^\dagger \mathcal{Z} | \varphi \rangle + \langle \varphi | \mathcal{Z} | \varphi \rangle^3 - \langle \varphi | \mathcal{Z}^\dagger | \varphi \rangle^2 \langle \varphi | \mathcal{Z} | \varphi \rangle = 0. \quad (2.80)$$

This equation can be interpreted by observing the Hartree evolution (2.70). Using this equation one can compute the time derivative of the expectation value of the operator $\mathcal{Z}$:

$$i\partial_t \langle \phi | \mathcal{Z} | \phi \rangle = \langle \phi | \mathcal{Z} | \phi \rangle - \langle \phi | \mathcal{Z}^\dagger \mathcal{Z} | \phi \rangle - \langle \phi | \mathcal{Z} | \phi \rangle^3 + \langle \phi | \mathcal{Z}^\dagger | \phi \rangle^2 \langle \phi | \mathcal{Z} | \phi \rangle. \quad (2.81)$$

Then, the condition (2.80) implies that $\partial_t \langle \phi | \mathcal{Z} | \phi \rangle|_{t=0} = 0$.

We can write explicitly this condition in terms of the variables $|\eta\rangle = C^{-1}|\varphi\rangle$ and α :

$$\begin{aligned} 0 = & 2(|\eta_0|^2 - |\eta_1|^2) \left(\text{Re}(\alpha^* \eta_0 \eta_1^*) + \text{Im}(\alpha^* \eta_0 \eta_1^*)^2 \right) \\ & + i \text{Im}(\alpha^* \eta_0 \eta_1^*) \left(|\eta_0|^2 + |\eta_1|^2 - 2(|\eta_0|^2 - |\eta_1|^2)^2 \right) \end{aligned} \quad (2.82)$$

One can observe in the numerical examples that the instance simulated in Figure 2.5b satisfies this condition and indeed the Hartree approximation works, while for the instances simulated in Figure 2.5c and Figure 2.5a this condition is not satisfied and the approximation fails.

2.4 Single-particle Hamiltonian

In this section, we are going to consider the last example of a non-Hermitian mean-field Hamiltonian. Lets consider the case where there is no interaction term $A^{(2)} = 0$. If the initial state is a pure product state $|\Psi^{(N)}(0)\rangle = |\varphi\rangle^{\otimes N}$, then the evolution is trivial and the mean-field approximation is exact for any single-particle operator. Indeed, the Schrodinger evolution (2.2) factorized completely

$$|\Psi^{(N)}(t)\rangle = \left(e^{-iA^{(1)}t}|\varphi\rangle\right)^{\otimes N}, \quad (2.83)$$

and then the normalized single-particle reduced density matrix can be written exactly as the projector on the solution of the Hartree equation (2.10),

$$\hat{\rho}^{(1)}(t) = \frac{e^{-iA^{(1)}t}|\varphi\rangle\langle\varphi|e^{iA^{(1)\dagger}t}}{\langle\varphi|e^{i2\text{Im}(A^{(1)})t}|\varphi\rangle} = |\phi(t)\rangle\langle\phi(t)|. \quad (2.84)$$

When we consider an initial state that is not completely concentrated on the initial Hartree solution, then the evolution is not trivial anymore. Motivated by the Hermitian case, lets consider an initial N -particle state given by

$$|\Psi^{(N)}(0)\rangle = \sum_{n=0}^N \alpha_n(0) |\varphi\rangle^{\otimes N-n} \otimes_s |\varphi_{\perp}\rangle^{\otimes n}, \quad (2.85)$$

for some normalized distribution $\sum_{n=0}^N |\alpha_n(0)|^2 = 1$. Motivated on the Hermitian case, assuming that the initial state corresponds to some condensate state. We considered two types of condensates, the polynomial condensate follows the distribution

$$\alpha_n^{\text{poly}}(0) \propto \frac{1}{(n+1)^r}. \quad (2.86)$$

for some $r > 0$, and the exponential condensate follows the distribution

$$\alpha_n^{\text{exp}}(0) \propto e^{-\beta n}, \quad (2.87)$$

for some $\beta > 0$.

We assume that $A^{(1)}$ is diagonalizable, then we can consider it is diagonal by fixing the desired basis. If it is diagonal, the Hermitian and anti-Hermitian part commutes and if

we apply a Hermitian evolution to an initial condensate it preserves the same distribution for the α_n over time, this follows from the discussion on the chapter 1 for the polynomial concentration, and it follows from the chapter 3 for the exponential concentration. Then we can focus only on the anti-Hermitian part by considering

$$A^{(1)} = iD = i \begin{pmatrix} \lambda_0 & 0 \\ 0 & \lambda_1 \end{pmatrix}. \quad (2.88)$$

The Hartree equation is immediately solvable

$$|\phi(t)\rangle = \frac{1}{\gamma(t)} e^{Dt} |\varphi\rangle. \quad (2.89)$$

where $\gamma(t) := \|e^{Dt}|\varphi\rangle\|$. But observe that since the evolution is not Hermitian, then it mixed the orthogonal states. Lets define $|\phi_\perp(t)\rangle$ as the continuous time evolving normalized vector such that at $t = 0$ it is equal to $|\varphi_\perp\rangle$ and it is always orthogonal to $|\phi(t)\rangle$. Define also $\gamma_\perp(t) := \|e^{Dt}|\varphi_\perp\rangle\|$, and the following angle

$$\sin(\theta(t)) := \langle \hat{\phi}(t) | e^{Dt} |\varphi_\perp\rangle \gamma_\perp(t)^{-1}, \quad \cos(\theta(t)) := \langle \hat{\phi}(t)_\perp | e^{Dt} |\varphi_\perp\rangle \gamma_\perp(t)^{-1}. \quad (2.90)$$

Then initial orthogonal states do not stay orthogonals

$$e^{Dt} |\varphi_\perp\rangle = \gamma_\perp(t) (\sin(\theta(t)) |\phi(t)\rangle + \cos(\theta(t)) |\phi_\perp(t)\rangle). \quad (2.91)$$

The evolution of the N -particle wave function is given by

$$|\Psi^{(N)}(t)\rangle = \sum_{n=0}^N \alpha_n(0) (e^{Dt} |\varphi\rangle)^{\otimes N-n} \otimes_s (e^{Dt} |\varphi_\perp\rangle)^{\otimes n}, \quad (2.92)$$

Using the equation (2.89) and (2.91), we can expand the unnormalized vector $|\Psi^{(N)}(t)\rangle$ in the tensor product base of $|\phi(t)\rangle, |\phi_\perp(t)\rangle$,

$$|\Psi^{(N)}(t)\rangle = \sum_{n=0}^N \alpha_n(t) |\phi(t)\rangle^{\otimes N-n} \otimes_s |\phi_\perp(t)\rangle^{\otimes n}, \quad (2.93)$$

with coefficients

$$\alpha_n(t) = \gamma^N \cos(\theta)^n \sum_{l=0}^{N-n} \sin(\theta)^l \alpha_{n+l}(0) \left(\frac{\gamma_\perp}{\gamma} \right)^{n+l} \binom{n+l}{n}. \quad (2.94)$$

This coefficients are not normalized due to the non unitary evolution. Nonetheless, we can interpret the distribution

$$P_n(t) := \frac{|\alpha_n(t)|^2}{\sum_m |\alpha_m(t)|^2}, \quad (2.95)$$

as the probability of finding n particles outside of the condensate. Using the expression (2.93) we can compute the unnormalized reduced density matrix and it is given by

$$\begin{aligned} \rho^{(1)}(t) = & \sum_{k=0}^{N-1} |\alpha_k(t)|^2 \frac{N-k}{N} |\phi(t)\rangle\langle\phi(t)| + \sum_{k=1}^N \alpha_k(t) \alpha_{k-1}^*(t) \sqrt{\frac{k(N-k+1)}{N^2}} |\phi_\perp(t)\rangle\langle\phi(t)| \\ & + \sum_{k=1}^N \alpha_k^*(t) \alpha_{k-1}(t) \sqrt{\frac{k(N-k+1)}{N^2}} |\phi(t)\rangle\langle\phi_\perp(t)| + \sum_{k=1}^N |\alpha_k(t)|^2 \frac{k}{N} |\phi_\perp(t)\rangle\langle\phi_\perp(t)|. \end{aligned} \quad (2.96)$$

Numerical results

In order to test the validity of the mean-field approximation, we compute numerically the infidelity (2.12) between the Hartree state (2.89) and the normalized reduced density matrix $\hat{\rho}^{(1)}(t)$. From (2.96) we obtain the infidelity

$$I = \frac{\sum_{k=0}^{N-1} |\alpha_k(t)|^2 \frac{k}{N}}{\sum_{k=0}^{N-1} |\alpha_k(t)|^2} = \left\langle \frac{k}{N} \right\rangle_{P(t)}. \quad (2.97)$$

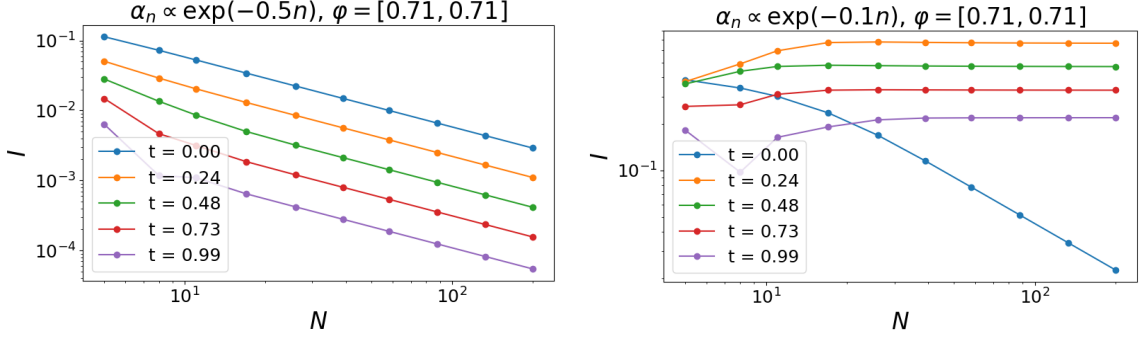
We chose the eigenvalues of the single-particle operator $\lambda_0 = 1, \lambda_1 = -1$ and fix the initial Hartree state $\varphi = (1/\sqrt{2}, 1/\sqrt{2})$. These numerical results are plotted in Figure 2.6 for three different instances, where we plot the infidelity as function of N for fix values of time.

We observed in Figure 2.6a, where we have an exponential condensation (2.87) with exponent $\beta = 0.5$, that the infidelity converges to zero, but this is not true for the polynomial concentration (Figure 2.6c) or the exponential concentration with smaller exponent $\beta = 0.1$ (Figure 2.6b). At $t = 0$, since the evolution does not have any effect yet, we have convergence of the infidelity in all the cases.

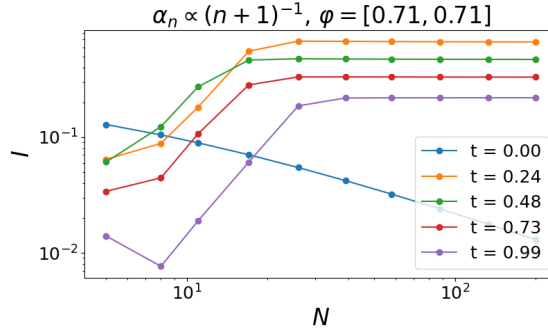
We interpret these results by observing that (2.97) converges to zero if the distribution is concentrated in zero, i.e. if the distribution preserves the exponential or the polynomial concentration. From the examples before, in order to preserve the concentration it is necessarily to have an exponential control with a sufficient large-negative coefficient of the initial distribution.

2.5 Lindblad evolution

Motivated by the algorithm discussed in subsection 1.4.2 for linearizing nonlinear differential equations using the mean-field approximation [33], but after showing that the approximation can fail for non-Hermitian Hamiltonians, we propose a different approach to the problem. Linearize the nonlinear differential equation by mapping it into a mean-field



(a) Initial exponential concentration with coefficient $\beta = 0.5$. (b) Initial exponential concentration with coefficient $\beta = 0.1$.



(c) Initial polynomial concentration with coefficient $r = 1$.

Figure 2.6: Infidelity between the Hartree state and the single-particle reduced density matrix for a mean-field Hamiltonian with single-particle operator (2.88) with eigenvalues $\lambda_0 = 1, \lambda_1 = -1$. Plot in log-log scale. It suggest that the validity of the mean-field approximation depend on having exponential control, with large enough exponent, on the initial distribution.

open quantum system and simulate the corresponding system in a quantum computer. Measurements of single-particle observables on the simulated system will approximate the corresponding measurements on the nonlinear system.

In this section, we are going to study the class of effective equations that arise from a mean-field approximation of an open quantum system. We will show that any first-order differential equation with polynomial nonlinearity can be obtained as an effective equation from a mean-field open quantum system, under the standard assumption that given an initial coherent state, the evolved state remains approximately coherent. This assumption is not rigorous in general, but it has been proven for different systems, such as the one proven by [68] and discussed in chapter 1. This proves that the linearization of the proposed

algorithm can be done.

Open quantum systems can be efficiently simulated following the algorithms proposed in [138–140]. It remains an open problem to compute explicit bounds for the rate of convergence of the mean-field open quantum system into the solution of the effective nonlinear equation. These bounds are required in order to know the error of the algorithm as a function of the number of particles simulated and therefore the running time.

Consider the normalized vector $\varphi \in \mathbb{C}^d$ and the initial coherent state with an average number of particles N defined by

$$a_i|\sqrt{N}\varphi\rangle = \sqrt{N}\varphi_i|\sqrt{N}\varphi\rangle. \quad (2.98)$$

The initial density matrix is then given by $\rho_N(0) = |\sqrt{N}\varphi\rangle\langle\sqrt{N}\varphi|$.

In order to generalize the construction of the mean-field Hamiltonian to interactions with an arbitrary number of particles, and preserving the scaling that keeps the Hamiltonian extensive in the number of particles, we define the following basis for the operators on the Fock space:

$$\mathcal{B}_N = \left\{ \frac{a_{\underline{l}}^\dagger a_{\underline{k}}}{N^{\frac{|\underline{l}|+|\underline{k}|}{2}-1}} : \underline{l}, \underline{k} \in \mathbb{N}^d \right\}. \quad (2.99)$$

The scaling with N is chosen such that $\text{Tr}(V\rho(0)) = \mathcal{O}(N) \forall V \in \mathcal{B}_N$. The notation is as follows: elements $\underline{l} \in \mathbb{N}^d$ are d -tuples of natural numbers including zero, of the form $\underline{l} = (l_1, \dots, l_d)$, and $|\underline{l}| = \sum_j l_j$. When they are a subscript of annihilation operators, the notation is

$$a_{\underline{l}} = a_1^{l_1} \dots a_d^{l_d}, \quad \forall \underline{l} = (l_1 \dots l_d) \in \mathbb{N}^d. \quad (2.100)$$

Let us define the Lindbladian operator, similarly to (1.40), acting on density matrices as

$$\mathcal{L}(\rho) = -i[H, \rho] + \frac{1}{N}\mathcal{D}(\rho), \quad (2.101)$$

where H describes the Hermitian evolution and is defined as

$$H := \sum_{V \in \mathcal{B}_N} p_V V, \quad (2.102)$$

with coefficients $p_{V^\dagger} = p_V^*$, and a dissipation operator defined as

$$\mathcal{D}(\rho) := \sum_{U, V \in \mathcal{B}_N} M_{U, V} \left(U \rho V^\dagger - \frac{1}{2} \{V^\dagger U, \rho\} \right). \quad (2.103)$$

The operator $\mathcal{D}$ is a valid dissipator if the matrix of coefficients M is positive semi-definite, in particular M is Hermitian, so it satisfies $M_{U, V} = M_{V, U}^*$. The scaling of the elements in $\mathcal{B}_N$ and the prefactor $1/N$ in (2.101) are chosen such that $\text{Tr}(\mathcal{L}(\rho(0))) = \mathcal{O}(N)$.

We consider the many-particle evolution given by the GKSL equation,

$$\begin{cases} \partial_t \rho_N(t) = \mathcal{L}(\rho_N(t)) \\ \rho_N(0) = |\sqrt{N}\varphi\rangle\langle\sqrt{N}\varphi| \end{cases} \quad (2.104)$$

Assuming that the evolution preserves the coherent state structure in the large N limit, we have $\rho_N(t) \approx |\sqrt{N}\phi(t)\rangle\langle\sqrt{N}\phi(t)|$ for some $\phi(t) \in \mathbb{C}^d$, and we want to find the Hartree equation describing the time evolution of $\phi(t)$. Using the definition (2.98) of a coherent state, we can compute the components of the vector as $\phi_j(t) = \text{Tr}(a_j \rho(t))/\sqrt{N} \forall j = 1 \dots d$, which satisfies the equation

$$\partial_t \phi_j(t) = \frac{1}{\sqrt{N}} \text{Tr} \left(\left(-i \sum_V p_V [a_j, V] + \frac{1}{2} \sum_{U,V} M_{U,V} (V^\dagger [a_j, U] - [a_j, V^\dagger] U) \right) \rho_N(t) \right). \quad (2.105)$$

Now we show that, in the limit of large N , this equation describes the Hartree equation for open quantum systems. Each of the operators $V \in \mathcal{B}_N$ represents some monomial in creation and annihilation operators indexed by some pair of multi-indices $\underline{l}, \underline{k} \in \mathbb{N}^d$.

Consider the following commutators,

$$\left[a_j, \frac{a_{\underline{l}}^\dagger a_{\underline{k}}}{N^{\frac{|\underline{l}|+|\underline{k}|-1}{2}}} \right] = l_j \frac{a_{\underline{l}-\underline{e}_j}^\dagger a_{\underline{k}}}{N^{\frac{|\underline{l}|+|\underline{k}|-1}{2}}}. \quad (2.106)$$

We are using the notation $\underline{e}_j := (0, \dots, 1, \dots, 0) \in \mathbb{N}^d$, and we define the difference between two multi-indexes as the difference element by element. It is well defined if the result has all positive elements. More precisely, let $\underline{l}, \underline{k} \in \mathbb{N}^d$, if $l_j \geq k_j \forall j = 1 \dots d$, we say that $\underline{l} \supseteq \underline{k}$ and we can define $\underline{l} - \underline{k} = (l_1 - k_1, \dots, l_d - k_d) \in \mathbb{N}^d$. In the context of (2.106), $\underline{l} - \underline{e}_j = (l_1, \dots, l_j - 1, \dots, l_d)$. Using (2.106) to compute the commutators in equation (2.105), we get

$$\begin{aligned} \partial_t \phi_j(t) = & \text{Tr} \left(-i \sum_{\underline{l}, \underline{k}} p_{\underline{l}, \underline{k}} l_j \frac{a_{\underline{l}-\underline{e}_j}^\dagger a_{\underline{k}}}{N^{\frac{|\underline{l}|+|\underline{k}|-1}{2}}} \rho(t) \right) \\ & + \text{Tr} \left(\sum_{\underline{m}, \underline{n}, \underline{s}, \underline{t}} M_{\underline{m}, \underline{n}, \underline{s}, \underline{t}} \frac{(m_j a_{\underline{l}}^\dagger a_{\underline{s}} a_{\underline{m}-\underline{e}_j}^\dagger a_{\underline{n}} - t_j a_{\underline{l}-\underline{e}_j}^\dagger a_{\underline{s}} a_{\underline{m}}^\dagger a_{\underline{n}})}{2N^{\frac{|\underline{s}|+|\underline{t}|+|\underline{m}|+|\underline{n}|-1}{2}}} \rho(t) \right). \end{aligned} \quad (2.107)$$

Now we use the assumption that the evolved state is coherent, and the trace property

$$\text{Tr} \left(a_{\underline{l}}^\dagger a_{\underline{k}} \rho(t) \right) = N^{\frac{|\underline{l}|+|\underline{k}|-1}{2}} \phi^*(t)^{\underline{l}} \phi(t)^{\underline{k}}, \quad (2.108)$$

where the notation, using multi-index in the exponent of a vector, is $\phi(t)^{\underline{k}} = \phi_1(t)^{k_1} \dots \phi_d(t)^{k_d}$ and equivalently for the complex conjugate $\phi^*(t)^{\underline{l}} = \phi_1^*(t)^{l_1} \dots \phi_d^*(t)^{l_d}$. In order to apply

(2.108), it is necessary to have the operators in normal order i.e., all creation operators on the left of the annihilation operators. This is not true for the second line of (2.107) so we have to put every term in normal order. The extra terms generated by non-trivial commutators have a smaller number of operators, and then they will scale at least with a relative factor N^{-1} with respect to the term with all the creation/annihilation operators. This scaling argument allows us to write every term in normal order and all the corrections will vanish in the large N limit. Then, equation (2.107) can be approximated by the Hartree equation for open quantum systems,

$$\partial_t \phi_j(t) = -i \sum_{\underline{l}, \underline{k}} p_{\underline{l}, \underline{k}} l_j \phi^*(t)^{\underline{l} - \underline{e}_j} \phi(t)^{\underline{k}} + \sum_{\underline{m}, \underline{n}, \underline{s}, \underline{t}} M_{\underline{m}, \underline{n}, \underline{s}, \underline{t}} \frac{(m_j - t_j)}{2} \phi^*(t)^{\underline{t} + \underline{m} - \underline{e}_j} \phi(t)^{\underline{s} + \underline{n}}. \quad (2.109)$$

The following result proves that any first-order differential equation with polynomial nonlinearity can be written in this form.

Lemma 2.5.1 (Expressivity of the Hartree equation of open systems). *Let $\phi(t) \in \mathbb{C}^d$ be a time dependent vector satisfying the differential equation*

$$\partial_t \phi(t) = F(\phi(t)), \quad (2.110)$$

where $F : \mathbb{C}^d \rightarrow \mathbb{C}^d$ is a polynomial vector field of arbitrary degree. Then, there exist some coefficients $p_{\underline{l}, \underline{k}} \in \mathbb{C}$ satisfying the Hermiticity condition

$$p_{\underline{l}, \underline{k}} = p_{\underline{k}, \underline{l}}^* \quad \forall \underline{l}, \underline{k} \in \mathbb{N}^d, \quad (2.111)$$

and coefficients $M_{\underline{m}, \underline{n}, \underline{s}, \underline{t}} \in \mathbb{C}$ satisfying the Hermiticity condition

$$M_{\underline{m}, \underline{n}, \underline{s}, \underline{t}} = M_{\underline{s}, \underline{t}, \underline{m}, \underline{n}}^*, \quad \forall \underline{m}, \underline{n}, \underline{s}, \underline{t} \in \mathbb{N}^d, \quad (2.112)$$

and the positivity condition

$$\sum_{\underline{m}, \underline{n}, \underline{s}, \underline{t}} \alpha_{\underline{m}, \underline{n}}^* M_{\underline{m}, \underline{n}, \underline{s}, \underline{t}} \alpha_{\underline{s}, \underline{t}} \geq 0 \quad \forall \alpha_{\underline{m}, \underline{n}} \in \mathbb{C}, \quad (2.113)$$

such that the equation (2.110) can be written in the form (2.109).

Proof. Given F , a polynomial vector field of arbitrary degree, and a vector $\phi \in \mathbb{C}^d$ we can write the j -th component of $F(\phi)$ as

$$F(\phi)_j = \sum_{\underline{l}, \underline{k}} F_{\underline{l}, \underline{k}}^{(j)} \phi^{*l} \phi^{\underline{k}}, \quad (2.114)$$

for some coefficients $F_{\underline{l},\underline{k}}^{(j)} \in \mathbb{C}$. By relabeling the dummy multi-indices $\underline{t} + \underline{m} \rightarrow \underline{l}$ and $\underline{s} + \underline{n} \rightarrow \underline{k}$, equation (2.109) is written as:

$$\partial_t \phi_j(t) = \sum_{\underline{l},\underline{k}} \left(-il_j p_{\underline{l},\underline{k}} + \frac{1}{2} \sum_{\underline{t} \subseteq \underline{l}} \sum_{\underline{s} \subseteq \underline{k}} (l_j - 2t_j) M_{\underline{l}-\underline{t},\underline{k}-\underline{s},\underline{s},\underline{t}} \right) \phi^*(t)^{\underline{l}-\underline{e}_j} \phi(t)^{\underline{k}}. \quad (2.115)$$

We will show that any set of coefficients $F_{\underline{l},\underline{k}}^{(j)}$ can be written as in (2.115)

Let us first rewrite the problem in order to lift the Hermiticity and positivity restrictions. Observe that the coefficients in (2.109) and (2.115) are invariant under the transformation $M_{\underline{m},\underline{n},\underline{s},\underline{t}} \rightarrow -M_{\underline{t},\underline{s},\underline{n},\underline{m}}$ for any $\underline{m}, \underline{n}, \underline{s}, \underline{t} \in \mathbb{N}^d$. We lift now the positivity condition and we will use this observation at the end of the proof to show that the result holds also for positive matrices. In order to work with arbitrary coefficients that do not satisfy the Hermiticity condition, we can replace

$$\begin{aligned} p_{\underline{l},\underline{k}} &\rightarrow \frac{1}{2} \left(\tilde{p}_{\underline{l},\underline{k}} + \tilde{p}_{\underline{k},\underline{l}}^* \right), \\ M_{\underline{m},\underline{n},\underline{s},\underline{t}} &\rightarrow \frac{1}{2} \left(\tilde{M}_{\underline{m},\underline{n},\underline{s},\underline{t}} + \tilde{M}_{\underline{s},\underline{t},\underline{m},\underline{n}}^* \right). \end{aligned} \quad (2.116)$$

From now on, $\tilde{M}_{\underline{m},\underline{n},\underline{s},\underline{t}}$ and $\tilde{p}_{\underline{k},\underline{l}}$ are arbitrary complex numbers.

Given the vector field F , we should solve the following set of equations,

$$F_{\underline{l}-\underline{e}_j,\underline{k}}^{(j)} = -\frac{i}{2} (\tilde{p}_{\underline{l},\underline{k}} + \tilde{p}_{\underline{k},\underline{l}}^*) l_j + \frac{1}{4} \sum_{\underline{s} \subseteq \underline{k}} \sum_{\underline{t} \subseteq \underline{l}} \left(\tilde{M}_{\underline{l}-\underline{t},\underline{k}-\underline{s},\underline{s},\underline{t}} + \tilde{M}_{\underline{s},\underline{t},\underline{l}-\underline{t},\underline{k}-\underline{s}}^* \right) (l_j - 2t_j) \quad \forall l_j > 0. \quad (2.117)$$

Since $F_{\underline{l},\underline{k}}^{(j)}$ are complex-valued, we have to consider their conjugate variables

$$F_{\underline{l}-\underline{e}_j,\underline{k}}^{(j)*} = \frac{i}{2} (\tilde{p}_{\underline{l},\underline{k}}^* + \tilde{p}_{\underline{k},\underline{l}}) l_j + \frac{1}{4} \sum_{\underline{s} \subseteq \underline{k}} \sum_{\underline{t} \subseteq \underline{l}} \left(\tilde{M}_{\underline{l}-\underline{t},\underline{k}-\underline{s},\underline{s},\underline{t}}^* + \tilde{M}_{\underline{s},\underline{t},\underline{l}-\underline{t},\underline{k}-\underline{s}} \right) (l_j - 2t_j) \quad \forall l_j > 0. \quad (2.118)$$

The first observation that will simplify the analysis is that we can divide these quantities into groups that share the same variables. The set of $F_{\underline{l}-\underline{e}_j,\underline{k}}^{(j)}, F_{\underline{k}-\underline{e}_j,\underline{l}}^{(j)*}$ for fixed $\underline{l}, \underline{k}$ and for all $j = 1, \dots, d$ are the only terms that depend on $\tilde{p}_{\underline{l},\underline{k}}, \tilde{p}_{\underline{k},\underline{l}}^*$, and $\{\tilde{M}_{\underline{a},\underline{b},\underline{c},\underline{d}}, \tilde{M}_{\underline{c},\underline{d},\underline{a},\underline{b}}^* : \underline{a} + \underline{d} = \underline{l}, \underline{b} + \underline{c} = \underline{k}\}$. This way, we have reduced the problem to a smaller set of equations with smaller number of variables. Furthermore, fix some q such that $l_q > 0$. Then, for every $j \neq q$ such that $l_j > 0$ we define

$$I_{\underline{l},\underline{k}}^{(j,q)} := F_{\underline{l}-\underline{e}_j,\underline{k}}^{(j)} l_q - F_{\underline{l}-\underline{e}_q,\underline{k}}^{(q)} l_j = \frac{1}{2} \sum_{\underline{s} \subseteq \underline{k}} \sum_{\underline{t} \subseteq \underline{l}} \left(\tilde{M}_{\underline{l}-\underline{t},\underline{k}-\underline{s},\underline{s},\underline{t}} + \tilde{M}_{\underline{s},\underline{t},\underline{l}-\underline{t},\underline{k}-\underline{s}}^* \right) (t_q l_j - t_j l_q). \quad (2.119)$$

Fix some r such that $k_r > 0$. Then, for every $u \neq r$ such that $k_u > 0$ define

$$I_{\underline{k}, \underline{l}}^{(u,r)*} := F_{\underline{k}-\underline{e}_u, \underline{l}}^{(u)*} k_r - F_{\underline{k}-\underline{e}_r, \underline{l}}^{(r)*} k_u = \frac{1}{2} \sum_{\underline{s} \subseteq \underline{k}} \sum_{\underline{t} \subseteq \underline{l}} \left(\tilde{M}_{\underline{l}-\underline{t}, \underline{k}-\underline{s}, \underline{s}, \underline{t}} + \tilde{M}_{\underline{s}, \underline{t}, \underline{l}-\underline{t}, \underline{k}-\underline{s}}^* \right) (s_r k_u - s_u k_r). \quad (2.120)$$

Consider the set of equations for fixed $\underline{l}, \underline{k}$:

$$\begin{cases} F_{\underline{l}-\underline{e}_q, \underline{k}}^{(q)} &= -\frac{i}{2} (\tilde{p}_{\underline{l}, \underline{k}} + \tilde{p}_{\underline{k}, \underline{l}}^*) l_q + \sum_{\underline{s} \subseteq \underline{k}} \sum_{\underline{t} \subseteq \underline{l}} \frac{1}{4} \left(\tilde{M}_{\underline{l}-\underline{t}, \underline{k}-\underline{s}, \underline{s}, \underline{t}} + \tilde{M}_{\underline{s}, \underline{t}, \underline{l}-\underline{t}, \underline{k}-\underline{s}}^* \right) (l_q - 2t_q) \\ F_{\underline{k}-\underline{e}_r, \underline{l}}^{(r)*} &= \frac{i}{2} (\tilde{p}_{\underline{l}, \underline{k}} + \tilde{p}_{\underline{k}, \underline{l}}^*) k_r - \sum_{\underline{s} \subseteq \underline{k}} \sum_{\underline{t} \subseteq \underline{l}} \frac{1}{4} \left(\tilde{M}_{\underline{l}-\underline{t}, \underline{k}-\underline{s}, \underline{s}, \underline{t}} + \tilde{M}_{\underline{s}, \underline{t}, \underline{l}-\underline{t}, \underline{k}-\underline{s}}^* \right) (k_r - 2s_r) \\ I_{\underline{l}, \underline{k}}^{(j,q)} &= \sum_{\underline{s} \subseteq \underline{k}} \sum_{\underline{t} \subseteq \underline{l}} \frac{1}{4} \left(\tilde{M}_{\underline{l}-\underline{t}, \underline{k}-\underline{s}, \underline{s}, \underline{t}} + \tilde{M}_{\underline{s}, \underline{t}, \underline{l}-\underline{t}, \underline{k}-\underline{s}}^* \right) 2(t_q l_j - t_j l_q), \quad \forall j \neq q : l_j > 0 \\ I_{\underline{k}, \underline{l}}^{(u,r)*} &= \sum_{\underline{s} \subseteq \underline{k}} \sum_{\underline{t} \subseteq \underline{l}} \frac{1}{4} \left(\tilde{M}_{\underline{l}-\underline{t}, \underline{k}-\underline{s}, \underline{s}, \underline{t}} + \tilde{M}_{\underline{s}, \underline{t}, \underline{l}-\underline{t}, \underline{k}-\underline{s}}^* \right) 2(s_r k_u - s_u k_r), \quad \forall u \neq r : k_u > 0. \end{cases} \quad (2.121)$$

We want to show that for any F , we can find $\tilde{p}_{\underline{k}, \underline{l}}$ and $\tilde{M}_{\underline{m}, \underline{n}, \underline{s}, \underline{t}}$ such that this set of equations is satisfied. And this is equivalent to showing that the set of equations is linearly independent. They are linearly independent if the set of equations

$$\alpha_1 F_{\underline{l}-\underline{e}_q, \underline{k}}^{(q)} + \alpha_2 F_{\underline{k}-\underline{e}_r, \underline{l}}^{(r)*} + \sum_{j \neq q : l_j > 0} \gamma_j I_{\underline{l}, \underline{k}}^{(j,q)} + \sum_{u \neq r : k_u > 0} \beta_u I_{\underline{k}, \underline{l}}^{(u,r)*} = 0, \quad (2.122)$$

for all $\tilde{p}_{\underline{l}, \underline{k}}, \tilde{p}_{\underline{k}, \underline{l}}^*, \tilde{M}_{\underline{l}-\underline{t}, \underline{k}-\underline{s}, \underline{s}, \underline{t}}, \tilde{M}_{\underline{s}, \underline{t}, \underline{l}-\underline{t}, \underline{k}-\underline{s}}^*$, have the unique solution $\alpha_1, \alpha_2, \beta_u, \gamma_j = 0$. We can write these equations as

$$\begin{aligned} 0 &= -\frac{i}{2} (\tilde{p}_{\underline{l}, \underline{k}} + \tilde{p}_{\underline{k}, \underline{l}}^*) (l_q \alpha_1 - k_r \alpha_2) \\ &+ \sum_{\underline{s} \subseteq \underline{k}} \sum_{\underline{t} \subseteq \underline{l}} \left(\tilde{M}_{\underline{l}-\underline{t}, \underline{k}-\underline{s}, \underline{s}, \underline{t}} + \tilde{M}_{\underline{s}, \underline{t}, \underline{l}-\underline{t}, \underline{k}-\underline{s}}^* \right) \left(\alpha_1 (l_q - 2t_q) - \alpha_2 (k_r - 2s_r) \right) \\ &+ \sum_{j \neq q : l_j > 0} \gamma_j 2(t_q l_j - t_j l_q) + \sum_{u \neq r : k_u > 0} \beta_u 2(s_r k_u - s_u k_r), \end{aligned} \quad (2.123)$$

and since this holds for every $\tilde{p}_{\underline{l}, \underline{k}}, \tilde{p}_{\underline{k}, \underline{l}}^*, \tilde{M}_{\underline{l}-\underline{t}, \underline{k}-\underline{s}, \underline{s}, \underline{t}}, \tilde{M}_{\underline{s}, \underline{t}, \underline{l}-\underline{t}, \underline{k}-\underline{s}}^* : \underline{s} \subseteq \underline{k}, \underline{t} \subseteq \underline{l}$, then they must satisfy

$$\begin{cases} 0 = l_q \alpha_1 - k_r \alpha_2 \\ 0 = \alpha_1 (l_q - 2t_q) - \alpha_2 (k_r - 2s_r) + \sum_{j \neq q : l_j > 0} \gamma_j 2(t_q l_j - t_j l_q) + \sum_{u \neq r : k_u > 0} \beta_u 2(s_r k_u - s_u k_r). \end{cases} \quad (2.124)$$

Using the first equation, we can replace $\alpha_2 = \frac{l_q}{k_r} \alpha_1$ into the second one, then

$$0 = \frac{2}{k_r} \alpha_1 (s_r l_q - t_q k_r) + \sum_{j \neq q : l_j > 0} \gamma_j 2(t_q l_j - t_j l_q) + \sum_{u \neq r : k_u > 0} \beta_u 2(s_r k_u - s_u k_r). \quad (2.125)$$

Since this equation must hold for all valid sub-indices $\underline{t} \subseteq \underline{l}$ and $\underline{s} \subseteq \underline{k}$, we can isolate the coefficients by evaluating specific index configurations. Considering the equation (2.125) with $\underline{t} = \underline{0}$, $\underline{s} = \underline{k}$, we obtain that

$$0 = 2\alpha_1 l_q \Rightarrow \alpha_1 = \alpha_2 = 0. \quad (2.126)$$

Now look at the equation (2.125) with $\underline{s} = \underline{k}$, choose some $i \neq q : l_i > 0$ and set $t_j = \delta_{ij}$. We conclude that

$$0 = \gamma_i. \quad (2.127)$$

Finally choose some $i \neq r : k_i > 0$ and look at the equation (2.125) with $s_u = \delta_{iu}$. We find that

$$\beta_i = 0. \quad (2.128)$$

This proves that, given any polynomial vector field F , there are matrices M and p satisfying the Hermiticity condition such that equations (2.110) and (2.109) match. We can write a map such that $F = \Phi(p, M)$; this relation is linear in p and M and it is invariant under the transformation $M_{\underline{m}, \underline{n}, \underline{s}, \underline{t}} \rightarrow -M_{\underline{t}, \underline{s}, \underline{n}, \underline{m}}$. Then, if we consider the following positive semi-definite operator with coefficients $I_{\underline{m}, \underline{n}, \underline{s}, \underline{t}} = \lambda \delta_{\underline{m}, \underline{s}} \delta_{\underline{n}, \underline{t}}$, for some $\lambda > 0$, the symmetry implies that $F = \Phi(p, M) = \Phi(p, M + I)$. Taking λ large enough guaranties that $p, M + I$ is an Hermitian and positive semi-definite solution. $\square$

Remark 2.5.2. The set of equations generated considering only the dissipative part, ($p_{\underline{l}, \underline{k}} = 0$) also spans the whole set of possible equations. And this is coherent with the fact that the commutator term in (2.101) can always be absorbed in the dissipator term. If we consider only the dissipative part, we can consider the set of equations

$$\begin{cases} F_{\underline{l}-e_q, \underline{k}}^{(q)} &= \sum_{\underline{s} \subseteq \underline{k}} \sum_{\underline{t} \subseteq \underline{l}} \frac{1}{4} \left(\tilde{M}_{\underline{l}-\underline{t}, \underline{k}-\underline{s}, \underline{s}, \underline{t}} + \tilde{M}_{\underline{s}, \underline{t}, \underline{l}-\underline{t}, \underline{k}-\underline{s}}^* \right) (l_q - 2t_q) \\ F_{\underline{k}-e_r, \underline{l}}^{(r)*} &= - \sum_{\underline{s} \subseteq \underline{k}} \sum_{\underline{t} \subseteq \underline{l}} \frac{1}{4} \left(\tilde{M}_{\underline{l}-\underline{t}, \underline{k}-\underline{s}, \underline{s}, \underline{t}} + \tilde{M}_{\underline{s}, \underline{t}, \underline{l}-\underline{t}, \underline{k}-\underline{s}}^* \right) (k_r - 2s_r) \\ I_{\underline{l}, \underline{k}}^{(j, q)} &= \sum_{\underline{s} \subseteq \underline{k}} \sum_{\underline{t} \subseteq \underline{l}} \frac{1}{4} \left(\tilde{M}_{\underline{l}-\underline{t}, \underline{k}-\underline{s}, \underline{s}, \underline{t}} + \tilde{M}_{\underline{s}, \underline{t}, \underline{l}-\underline{t}, \underline{k}-\underline{s}}^* \right) 2(t_q l_j - t_j l_q), \quad \forall j \neq q : l_j > 0 \\ I_{\underline{k}, \underline{l}}^{(u, r)*} &= \sum_{\underline{s} \subseteq \underline{k}} \sum_{\underline{t} \subseteq \underline{l}} \frac{1}{4} \left(\tilde{M}_{\underline{l}-\underline{t}, \underline{k}-\underline{s}, \underline{s}, \underline{t}} + \tilde{M}_{\underline{s}, \underline{t}, \underline{l}-\underline{t}, \underline{k}-\underline{s}}^* \right) 2(s_r k_u - s_u k_r), \quad \forall u \neq r : k_u > 0 \end{cases} \quad (2.129)$$

The question about the independence of these equations leads to solving the system

$$\left\{ \begin{aligned} 0 &= \alpha_1 (l_q - 2t_q) - \alpha_2 (k_r - 2s_r) + \sum_{j \neq q : l_j > 0} \gamma_j 2(t_q l_j - t_j l_q) + \sum_{u \neq r : k_u > 0} \beta_u 2(s_r k_u - s_u k_r). \end{aligned} \right. \quad (2.130)$$

This is the same as the general case but with one fewer restriction. However, if we set $\underline{t} = \underline{l}$ $\underline{s} = \underline{k}$ we get the equation

$$0 = -\alpha_1 l_q + \alpha_2 k_r. \quad (2.131)$$

We recover the missing equation, then the system of equations is equivalent to the previous one and the only solution is still $\alpha_1, \alpha_2, \beta_u, \gamma_j = 0$.

2.6 Conclusions and perspectives

The main message of this chapter is that the Hartree equation does not always provide a good approximation to the evolution of the one-particle marginal state under a non-Hermitian many-body dynamics. We discussed how to derive the Hartree equation by using the BBGKY hierarchy and a factorized ansatz for the reduced density matrix. We showed that this heuristic approach does not capture the correct dynamics, the reason is that the non-Hermitian terms of the Hamiltonian amplify the interaction due to small correlations present in the many-body wavefunction that are not included in the Hartree equation. This phenomenon becomes explicit when comparing the second time derivative of the Hartree solution and of the single-particle reduced density matrix, and furthermore, the condition that both second time derivatives match can be used as a necessary condition of the initial state for the success of the Hartree approximation.

We presented three examples to make explicit the new situations that appear for non-Hermitian Hamiltonians. First, we have considered a system of N bosonic qubits evolving with the purely anti-Hermitian Hamiltonian $\frac{i}{N-1} \sum_{i < j} Z_i Z_j$, starting from a pure product state, and we have computed an analytic expression for the limit as $N \rightarrow \infty$ of the one-particle marginal state. We have found that, for almost every initial condition, such a limit is pure but does not satisfy the non-Hermitian generalization of the Hartree equation. Therefore, the Hartree approximation fails even if the limit of the one-particle marginal state is pure. Furthermore, we have derived the correct effective evolution equation for the limiting one-particle wavefunction. This evolution differs from the Hartree equation by an explicit time dependence, and it matches the Hartree equation only at $t = 0$. Moreover, we have shown that there exists an initial condition such that the one-particle dynamics exhibits a finite critical time $t_c = \frac{1}{2}$. The limit for $N \rightarrow \infty$ of the one-particle marginal state is pure and satisfies the Hartree equation up to $t = \frac{1}{2}$, but for $t > \frac{1}{2}$ the limiting one-particle marginal state becomes mixed and the Hartree approximation breaks down.

Second, we have numerically studied a bosonic non-Hermitian mean-field Hamiltonian with real spectrum and we have shown that, also in this case, there are initial product states such that the time-evolved one-particle state does not converge to the solution of the Hartree equation in the limit $N \rightarrow \infty$.

Third, we considered an example where there is no interacting term in the Hamiltonian and the single-particle operator is not Hermitian. If the initial product state is completely factorized, the evolution is trivial and the Hartree approximation becomes exact; nonetheless, we simulated the case where the initial state is in a condensate state which is not

exactly factorized, but there is a probability distribution of having excited particles. In this case, we found that it is necessary to have an exponentially concentrated initial state for the Hartree approximation to succeed, while having a polynomial concentration is not enough.

Our findings motivate different research directions. The first one is to characterize the set of non-Hermitian Hamiltonians for which the Hartree approximation is valid given a pure factorized initial state. We already know that such a set includes non-interacting systems and arbitrary bosonic systems with Hermitian Hamiltonians. A hint for such a set can be given by the non-Hermitian Hamiltonians such that, at $t = 0$, the second time derivative of the one-particle marginal state matches the second time derivative of the solution of the Hartree equation.

The second possible direction is more challenging and consists of deriving a correct effective evolution equation for the one-particle marginal state. In this chapter, we have derived such an equation for the considered Hamiltonian (2.52). Since this equation includes an explicit time dependence despite the fact that the many-body Hamiltonian is time-independent, our findings suggest that a general framework to describe non-Hermitian dynamics of bosonic mean-field systems may need to include additional information not captured by the naive product-state ansatz. Establishing such a framework and clarifying its relationship to mean-field limits would significantly improve the reliability of mean-field models in both many-body quantum physics and quantum algorithm design.

Lastly, the failure of the Hartree approximation implies that the algorithm proposed in [33] cannot be applied to general nonlinear differential equations. We proposed to modify the linearization method used in this algorithm and to consider the mean-field regime of open quantum systems instead of non-Hermitian Hamiltonians. We took a first step in this direction by proving that any nonlinear Schrödinger differential equation with polynomial nonlinearity can be written as the mean-field effective equation of an open quantum system assuming that the state remains approximately coherent during the evolution. The convergence of the mean-field effective equation and how to simulate the corresponding many-body system are solved in the literature, and it remains an open problem to compute the explicit bounds on the convergence and use it to compute the running time of such algorithm.

Chapter 3

Exponential condensation

As discussed in the introduction and in chapter 1, there is a vast bibliography on the mathematical description of the mean-field regime and the macroscopic condensation on the Hartree solution.

We contribute to the analysis of condensation along the mean-field dynamics by proving that the probability of having n particles outside the condensate decays exponentially with n for any finite evolution time. This result strengthens previously known bounds of the type (1.18) or (1.22), which prove only a polynomial decay of such a probability, we will explain this probabilistic picture below.

Given the abstract mean-field Hamiltonian (6), we consider two physically relevant classes of mean-field models:

- Type (i) *Arbitrary bounded interactions*: we assume that the two-body interaction w is bounded, i.e. $\|w\| < \infty$, but otherwise arbitrary.
- Type (ii) *Unbounded interaction potentials*: we set $\mathfrak{h} = L^2(\mathbb{R}^3)$, $T = -\Delta$, and assume that the interaction is given by multiplication with a potential of the form $w(x, y) = V(x - y)$. The Hamiltonian is then given by (1) with $V_{ext} = 0$.

$$H^{(N)} = \sum_{i=1}^N -\Delta_{x_i} + \frac{1}{N-1} \sum_{1 \leq i < j \leq N} V(x_i - x_j). \quad (3.1)$$

The operator V satisfies the inequality

$$V^2 \leq D(1 - \Delta) \quad (3.2)$$

for some constant $D > 0$.

Mean-field models of type (i) naturally arise, for example, in the description of spin systems [15, 141], and Lipkin-Meshkov-Glick-type models [142]. In the continuum, bounded

interactions arise naturally as soft-core or regularized potentials of finite height, which are used to model effective interactions in ultracold atomic gases, for instance in Rydberg-dressed systems and related proposals for supersolid phases [143]. The Kac model and soft spheres can also be described by type (i) models [144].

Mean-field models with unbounded interaction potentials of type (ii) constitute a standard mathematical framework for the description of Bose–Einstein condensation, and the condition (3.2) is chosen in order to include the Coulomb potential; see for example [18].

3.1 Main results

We show that if the initial number of excitations is exponentially controlled, the property of exponential condensation is preserved for positive times. More precisely we consider an initial condensate state (7) satisfying

$$\langle \Psi^{(N)}(0), \exp(\beta \mathcal{N}_+(0)) \Psi^{(N)}(0) \rangle \leq C_\beta \quad (3.3)$$

for $\beta > 0$ and some $C_\beta > 0$ independent of N . The exponential control on the initial condition is justified by [145–147], where they show that it holds for the ground state of mean-field Hamiltonians. Then, we prove that in the large N limit,

$$\langle \Psi^{(N)}(t), \exp(\beta \mathcal{N}_+(t)) \Psi^{(N)}(t) \rangle = \mathcal{O}(1) \quad (3.4)$$

for $\beta \leq \beta_c(t)$ and suitable $\beta_c(t) > 0$ discussed below.

Since there are small technical differences for the two different types of models (i), (ii) we present two theorems describing the exponential condensation (3.4) in each case. We start by the type (i) models.

Theorem 3.1.1 (Exponential Condensation for bounded potentials). *Let w be an arbitrary bounded two-body interaction, let $\Psi^{(N)}(t) \in \text{Sym}^N \mathfrak{h}$ denote the solution to the Schrödinger equation (5) with initial data (7) satisfying the condensate condition (3.3). Furthermore, let $\phi(t)$ denote the solution to the Hartree equation (8) with initial data $\phi(0) \in \mathfrak{h}$.*

Then, the number of excitations $\mathcal{N}_+(t)$ defined by (1.19), satisfies

$$\left\langle \Psi^{(N)}(t), \exp(\beta \mathcal{N}_+(t)) \Psi^{(N)}(t) \right\rangle \leq C_\beta f(t, \beta) \quad (3.5)$$

for all $t \geq 0$ and $0 \leq \beta < \beta_c(t) = -\ln \tanh(3\|w\|t)$, where

$$f(t, \beta) = \left(\frac{1 - \tanh(3\|w\|t) e^{-\beta}}{1 - \tanh(3\|w\|t) e^\beta} \right)^{1/3}. \quad (3.6)$$

For models of type (ii) the condition (3.2) can be written in the integral form

$$\int_{x \in \mathbb{R}^3} V(x)^2 |\psi(x)|^2 dx \leq D \int_{x \in \mathbb{R}^3} \left(|\psi(x)|^2 + |\nabla \psi(x)|^2 \right) dx, \quad (3.7)$$

for any $\psi \in H^1(\mathbb{R}^3)$. The associated Hartree dynamics has a unique mild solution, and, moreover

$$\mathbb{V} := \sup_x \int |V(x-y)\phi(t,y)|^2 dy < \infty, \quad (3.8)$$

see for example [18]. In this setting, we prove exponential condensation of the form (3.4), too.

Theorem 3.1.2 (Exponential condensation for unbounded interaction potentials). *Let $\mathfrak{h} = L^2(\mathbb{R}^3)$, $T = -\Delta$ and w given by multiplication with a potential of the form $w(x,y) = V(x-y)$ satisfying (3.2), let $\Psi^{(N)}(t) \in \text{Sym}^N \mathfrak{h}$ denote the solution to the Schrödinger equation (5) with initial datum (7) satisfying the condensate condition (3.3). Furthermore, let $\phi(t)$ denote the solution to the Hartree equation (8) with initial datum $\phi(0) \in \mathfrak{h}$.*

Then, the number of excitations $\mathcal{N}_+$ defined by (1.19) satisfies

$$\left\langle \Psi^{(N)}(t), \exp(\beta \mathcal{N}_+(t)) \Psi^{(N)}(t) \right\rangle \leq C_\beta f(t, \beta) \quad (3.9)$$

for all $t \geq 0$ and for all $0 \leq \beta < \beta_c(t) = -\ln \tanh(6\mathbb{V}t)$, where

$$f(t, \beta) = \left(\frac{1 - \tanh(6\mathbb{V}t) e^{-\beta}}{1 - \tanh(6\mathbb{V}t)} e^\beta \right)^{1/3}. \quad (3.10)$$

Remark 3.1.3. We collect a few remarks on the constants $f(t, \beta)$ and $\beta_c(t)$ appearing in Theorem 3.1.1 and Theorem 3.1.2.

- (i) Since the bound $f(t, \beta)$ on the moment generating function of $\mathcal{N}_+(t)$ does not depend on the total number of particles N , the theorems indeed establishes exponential condensation in the sense of (3.4). Moreover, $f(0, \beta) = 1$ for all $\beta > 0$ and $f(t, 0) = 1$ for all $t \geq 0$. Hence, for the pairs $(0, \beta)$ and $(t, 0)$, the upper bound provided by the theorem coincides with the exact value of the corresponding quantity.
- (ii) We note that $\beta_c(t) > 0$ for all finite times, and therefore exponential condensation holds for any $t \geq 0$. The critical parameter $\beta_c(t)$ scales as $\mathcal{O}(\log(t^{-1}))$ for small times and as $\mathcal{O}(e^{-t})$ for large times.

Remark 3.1.4 (Probabilistic picture). As mentioned above, the number of excitations in the state $\Psi^{(N)}(t)$ can be interpreted as a random variable with distribution

$$\mathbb{P}_{\Psi^{(N)}(t)}[\mathcal{N}_+(t) = n] = \langle \Psi^{(N)}(t), \mathbf{1}_{\{\mathcal{N}_+(t)=n\}} \Psi^{(N)}(t) \rangle. \quad (3.11)$$

In this probabilistic picture, the theorems provide an upper bound on the moment generating function of $\mathcal{N}_+(t)$. As a consequence of Markov's inequality, we obtain

$$\mathbb{P}_{\Psi(N)(t)}[\mathcal{N}_+(t) > n] \leq C_\beta f(t, \beta) e^{-\beta n} \quad (3.12)$$

for all $\beta < \beta_c(t)$. Hence, the probability of finding more than n particles outside the condensate decays exponentially in n .

Comparison to the literature

As discussed in the introduction, our results fit into a broad body of literature on the analysis of Bose–Einstein condensation for mean-field models [13, 15, 17–19, 141, 148–156], as well as on the study of quantum fluctuations, i.e. particles outside the condensate, in such systems [24–32]; see also the review article [157]. Our results, however, complement the existing literature on mean-field dynamics by providing a stronger, exponential control of the number of excited particles. We remark that, for large times, the critical value β_c decays exponentially in time, and our bounds are consistent with earlier results on moment estimates for the number of excitations, which typically grow exponentially in time; see, for example, [18] under similar assumptions on the initial data and interaction potential.

Probabilistic picture

To the best of our knowledge, our work establishes the first bound on the moment generating function of the number of excitations along the many-body time evolution; see Remark 3.1.4. For mean-field models in the ground state, bounds on the moment generating function have been obtained earlier [145–147], and its asymptotic behavior has been analyzed more recently in [158]. From this perspective, our results provides a first step towards exponential control of excitations in the time-dependent setting.

Singular scaling regimes

From a physical point of view, the most relevant but mathematically most challenging setting is the analysis of singular interaction potentials in the so-called Gross-Pitaevskii regime. In this regime, the mean-field interaction potential V is replaced by an N -dependent potential $V_N = N^3 V(N\cdot)$, which scales with the total number of particles and converges, in the large-particle limit, to a δ -interaction. Remarkably, bounds [146, 147, 158] and asymptotic formulas for the moment generating function of the number of excitations in the ground state have been shown to remain valid even in this mathematically challenging regime. For the corresponding many-body dynamics, however, only bounds on the first moment of the number of excitations are currently known [159], while bounds on higher moments remain a challenging open problem.

3.2 Proof of the theorems

In this section, we prove Theorem 3.1.1 and Theorem 3.1.2. The idea for both proofs is the same: The goal is to prove that the function $g_N : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ given by

$$g_N(t, \beta) = \left\langle \Psi^{(N)}(t), \exp(\beta \mathcal{N}_+(t)) \Psi^{(N)}(t) \right\rangle. \quad (3.13)$$

satisfies a Gronwall type estimate of the form

$$\partial_t g_N(t, \beta) \leq \left(8K \sinh\left(\frac{\beta}{2}\right) + 2K \sinh(\beta) \right) \partial_\beta g_N(t, \beta) + 2 \sinh(\beta) K g_N(t, \beta). \quad (3.14)$$

where the constant $K > 0$ depends on the choice of the two-particle interaction. In fact, we shall prove that for the choice of bounded interactions, in Theorem 3.1.1, we have $K = \|w\|$, while for unbounded interactions, in Theorem 3.1.2, we have $K = 2\mathbb{V}$.

We split the proof in three steps: In the first step, in subsection 3.2.2, we compute the derivative of $\partial_t g_N(t, \beta)$ that works the same for both Theorems. In the second step, in subsection 3.2.3, we then derive an estimate of the form (3.14). As discussed before, the technical details of the bound depends on the choice of the two-particle interaction w and is therefore proven differently for both Theorems in section 3.2.3 and section 3.2.3. In the final third step in subsection 3.2.4, we perform a Gronwall-type argument to derive the final results in Theorem 3.1.1 and Theorem 3.1.2 from (3.14).

We will use the excitation map described in section 1.2. Since the definition (1.12) is not an explicit construction of the operator, before proceeding with the proof, we will show how to construct this mapping and give some useful properties.

3.2.1 Excitation map revisited

For the definition of the excitation map, we embed any N -particle wavefunction into the bosonic Fock space through $W_N : \text{Sym}^N \mathfrak{h} \rightarrow \mathcal{F}$ given by

$$W_N(\Psi^{(N)}) := \left(\bigoplus_{n=0}^{N-1} 0 \right) \oplus \Psi^{(N)} \oplus \left(\bigoplus_{n=0}^{N-1} 0 \right), \quad \text{and} \quad W_N^* \left(\bigoplus_{n=0}^{\infty} \psi^{(n)} \right) = \psi^{(N)} \quad (3.15)$$

where W_N^* denotes the adjoint of W_N . In particular, note that while $W_N^* W_N$ acts as the identity on $\text{Sym}^N \mathfrak{h}$, the adjoint $W_N W_N^*$ acts on $\mathcal{F}$ as a projector onto the subspace of N particles. Moreover, we define $Q_{N,t} : \mathcal{F} \rightarrow \mathcal{F}$ as the orthogonal projector from the full bosonic Fock space $\mathcal{F}$ on the orthogonal Fock space $\mathcal{F}_{\perp \phi(t)}^{\leq N}$ by

$$Q_{N,t} := \left(\bigoplus_{n=0}^N (1 - |\phi(t)\rangle \langle \phi(t)|)^{\otimes n} \right) \oplus \left(\bigoplus_{n=N+1}^{\infty} 0 \right). \quad (3.16)$$

Then, the excitation map defined in (1.12), can be explicitly written as

$$U_{N,t} = \sum_{n=0}^N Q_{N,t} \frac{a(\phi(t))^{N-n}}{\sqrt{(N-n)!}} W_N. \quad (3.17)$$

Note that in this picture, the number of excitations defined in (1.19) reads

$$W_N \mathcal{N}_+(t) W_N^* = \mathcal{N} - a^*(\phi(t))a(\phi(t)) = \sum_{i \in \mathbb{N}_+} a_i^* a_i, \quad (3.18)$$

where $\mathcal{N} = \sum_{i \in \mathbb{N}} a_i^* a_i$ is the number operator.

By construction, the excitation map $U_{N,t}$ maps any N -particle wavefunction into the orthogonal Fock space by destroying all particles in the Hartree wavefunction $e_0 = \phi(t)$. In particular note that the image of $U_{N,t}$ is the orthogonal Fock space $\mathfrak{S}(U_{N,t}) = \mathfrak{S}(Q_{N,t}) = \mathcal{F}_{\perp \phi(t)}^{\leq N}$, respecting the heuristics that an N -particle wavefunction can have at most N excitations outside the Hartree evolution. We can then define the initial excitations state

$$\Xi_N := U_{N,0} \Psi^{(N)}(0) = \bigoplus_{n=0}^N \xi^{(n)}. \quad (3.19)$$

Furthermore, the conjugate of the excitation map is given by

$$U_{N,t}^* = \sum_{n=0}^N W_N^* \frac{(a(\phi(t))^*)^{N-n}}{\sqrt{(N-n)!}} Q_{N,t}. \quad (3.20)$$

Since $U_{N,t}^* U_{N,t} = 1$ and $U_{N,t} U_{N,t}^* = Q_{N,t}$, the excitation map is a partial isometry.

The excitation map comes with nice properties, we write them in a slightly different form from [63], that will be more useful for our computations: It transforms the projected creation and destruction operators to

$$\begin{aligned} U_{N,t} W_N^* a_n^* W_{N-1} U_{N-1,t}^* &= \begin{cases} Q_{N,t} a_n^* Q_{N-1,t} & \forall n \geq 1 \\ Q_{N,t} \sqrt{N - \mathcal{N}} Q_{N-1,t} & n = 0 \end{cases} \\ U_{N-1,t} W_{N-1}^* a_n W_N U_{N,t}^* &= \begin{cases} Q_{N-1,t} a_n^* Q_{N,t} & \forall n \geq 1 \\ Q_{N-1,t} \sqrt{N - \mathcal{N}} Q_{N,t} & n = 0 \end{cases}. \end{aligned} \quad (3.21)$$

Lets prove the transformation of a_n by using the explicit construction of the adjoint excitation map (3.20). After plugging (3.20), we observe that we can simplify $W_{N-1}^* a_n W_N W_N^* = W_{N-1}^* a_n$, then

$$U_{N-1,t} W_{N-1}^* a_n W_N U_{N,t}^* = U_{N-1,t} W_{N-1}^* a_n \sum_{m=0}^N \frac{(a_0^*)^{N-m}}{\sqrt{(N-m)!}} Q_{N,t} \quad (3.22)$$

If $n > 0$, the creation and destruction operators commute, and furthermore we can write $a_n Q_{N,t} = Q_{N-1,t} a_n Q_{N,t}$. Then

$$U_{N-1,t} W_{N-1}^* a_n W_N U_{N,t}^* = U_{N-1,t} W_{N-1}^* \sum_{m=0}^N \frac{(a_0^*)^{N-m}}{\sqrt{(N-m)!}} Q_{N-1,t} a_n Q_{N,t} \quad (3.23)$$

Since W_{N-1}^* selects the sector of $N-1$ particles, the terms with $m=0$ vanish, and we are left with the operator $U_{N-1,t}^*$. Since $U_{N-1,t} U_{N-1,t}^* = Q_{N-1}$, it proves the case $n > 0$.

If $n = 0$ we use the commutation relations and $a_0 Q_{N,t} = 0$ to write

$$U_{N-1,t} W_{N-1}^* a_n W_N U_{N,t}^* = U_{N-1,t} W_{N-1}^* \sum_{m=0}^N \frac{(a_0^*)^{N-1-m}}{\sqrt{(N-1-m)!}} \sqrt{N-m} Q_{N,t}. \quad (3.24)$$

Since W_{N-1}^* selects the sector of $N-1$ particles and $N-1-m$ particles are in the Hartree state, then m is the number of orthogonal particles. Also, since the image of $Q_{N,t}$ has only orthogonal particles, we can replace $N-m$ by $N-\mathcal{N}$. We can then reconstruct the operator $U_{N-1,t}^*$ and use the identity $U_{N-1,t} U_{N-1,t}^* = Q_{N-1,t}$ to finish the proof.

Thus, in the limit of infinitely many particles, where we expect that the number of excitation is $\mathcal{O}(1)$, a particle created through $a_0 = a(\phi(t))$ along the Hartree evolution is effectively replaced by an $\mathcal{O}(\sqrt{N})$ quantity, while excitations orthogonal to the Hartree evolution, created through a_n^* with $n \geq 1$, are replaced by $\mathcal{O}(1)$ quantities. In physics this formal transformation is referred to as c-number substitution. Note that $U_{N,t}$ furthermore maps the projected number of excitations (3.18) to the number of particles operator on the orthogonal Fock space, i.e.

$$U_{N,t} \mathcal{N}_+(t) U_{N,t}^* = \sum_{n \geq 1} U_{N,t} W_N^* a_n^* W_{N-1} U_{N-1,t}^* U_{N-1,t} W_{N-1}^* a_n W_N U_{N,t}^* = \mathcal{N} Q_N, \quad (3.25)$$

where we used that $W_{N-1} U_{N-1,t}^* U_{N-1,t} W_{N-1}^* = 1$ on the image of $a_n W_N U_{N,t}^*$, similarly $Q_{N-1,t} = 1$ on the image of $a_n Q_{N,t}$ and $Q_{N,t}$ commutes with $\mathcal{N}$. The projected particle-number operator $\mathcal{N} = \sum_{i=0}^{\infty} a_i^* a_i$ (that is actually time independent) is mapped by the excitation map to

$$U_{N,t} W_N^* \mathcal{N} W_N U_{N,t}^* = \mathcal{N} Q_{N,t} + (N - \mathcal{N}) Q_{N,t} = N Q_{N,t}. \quad (3.26)$$

Since we are embedding the N -particle wavefunction into the bosonic Fock space through W_N defined in (3.15). For the analysis, we therefore also need to transform the Hamiltonian $H^{(N)}$ originally defined in (6) on the N -particle Hilbert space $\text{Sym}^N \mathfrak{h}$ to an operator on the Fock space: We recall that $H^{(N)}$ is defined as a sum of one-particle operators T_i and two-particle operators w_{ij} whose second quantization is defined as

$$d\Gamma(T) = \bigoplus_{n=1}^{\infty} \sum_{i=1}^n T_i, \quad d\Gamma(w) = \bigoplus_{n=2}^{\infty} \sum_{i < j} w_{ij}. \quad (3.27)$$

Thus, the N -particle Hamiltonian and the Hartree Hamiltonian act on the Fock space as

$$d\Gamma(H^{(N)}) = d\Gamma(T) + \frac{1}{N-1}d\Gamma(w), \quad \text{resp.} \quad d\Gamma(H_H^{\phi(t)}) = d\Gamma(T) + d\Gamma(w^{\phi(t)}). \quad (3.28)$$

We remark that the interaction potential can be written in terms of creation and annihilation operators

$$d\Gamma(w) = \frac{1}{2} \sum_{m,n,p,q \in \mathbb{N}} w_{mnpq} a_m^* a_n^* a_q a_p, \quad \text{and} \quad d\Gamma(w^{\phi(t)}) = \sum_{m,p \in \mathbb{N}} w_{m0p0} a_m^*, \quad (3.29)$$

where $w_{mnpq} = \langle e_m \otimes e_n, w e_p \otimes e_q \rangle$, recalling that, in abuse of notation we set $\phi(t) = e_0$, and the series converges strongly in any subspace of the Fock space with bounded number of particles. Furthermore, the matrix elements w_{mnpq} satisfy the following properties:

- (i) If w is Hermitian, then $w_{mnpq}^* = w_{pqmn}$.
- (ii) If w is symmetric under the exchange of particles, then $w_{mnpq} = w_{mnqp} = w_{nmpq} = w_{nmqp}$.

Now that we have all the ingredients, we proceed with the three steps of the proof.

3.2.2 Step 1

In this section, we derive an explicit expression for the time derivative of $g_N(t, \beta)$ defined in (3.13). Note that in fact, in the definition of $g_N(t, \beta)$ there are two quantities that depend on time: the many-body wavefunction $\Psi^{(N)}(t)$ and (in abuse of notation) the orthogonal number operator $\mathcal{N}_+(t)$. However, introducing the fluctuation dynamics

$$\mathcal{U}_N(t, 0) := U_{N,t} e^{-iH^{(N)}t} U_{N,0}^* \quad (3.30)$$

and using that by our choice of initial data (3.19), we have from (5) and the identity (3.25)

$$g_N(t, \beta) = \langle \mathcal{U}_N(t, 0) \Xi_N, \exp(\beta \mathcal{N}) \mathcal{U}_N(t, 0) \Xi_N \rangle. \quad (3.31)$$

Thus, we passed the time dependency of the expectation value to the fluctuations dynamics $\mathcal{U}_N(t; 0)$ only. The fluctuation dynamics satisfies

$$i\partial_t \mathcal{U}_N(t, 0) = \mathcal{L}_N(t) \mathcal{U}_N(t, 0), \quad (3.32)$$

with the evolution generator

$$\mathcal{L}_N(t) = (i\partial_t U_{N,t}) U_{N,t}^* + U_{N,t} H^{(N)} U_{N,t}^*. \quad (3.33)$$

In the following, we use the short-hand notation $\langle \cdot \rangle$ for the expectation value of any operator in the state $\mathcal{U}_N(t, 0) \Xi_N$. With this notation, the time derivative of g_N reads

$$\partial_t g_N(t, \beta) = -i \langle [\exp(\beta \mathcal{N}), \mathcal{L}_N(t)] \rangle. \quad (3.34)$$

To calculate the commutator, we first derive an explicit expression for the generator $\mathcal{L}_N(t)$ of the fluctuation dynamics (3.33) in terms of creation and annihilation operators. We start with the time derivative of the excitation map. We recall the definition of $U_{N,t}$ in (3.17). One can prove the following equations using the Hartree equation,

$$i\partial_t a(\phi(t)) = [d\Gamma(H_H^{\phi(t)}), a(\phi(t))], \quad \text{and} \quad i\partial_t Q_{N,t} = [d\Gamma(H_H^{\phi(t)}), Q_{N,t}], \quad (3.35)$$

then we find that

$$\begin{aligned} i\partial_t U_{N,t} &= \left[d\Gamma(H_H^{\phi(t)}), \sum_{n \in \mathbb{N}} Q_{N,t} \frac{a(\phi(t))^{N-n}}{\sqrt{(N-n)!}} \right] W_N \\ &= d\Gamma(H_H^{\phi(t)}) U_{N,t} - \left(\sum_{n \in \mathbb{N}} Q_{N,t} \frac{a(\phi(t))^{N-n}}{\sqrt{(N-n)!}} \right) d\Gamma(H_H^{\phi(t)}) W_N \\ &= d\Gamma(H_H^{\phi(t)}) U_{N,t} - U_{N,t} W_N^* d\Gamma(H_H^{\phi(t)}) W_N. \end{aligned} \quad (3.36)$$

In the last step, we used that $W_N W_N^*$ acts as the identity in the image of W_N , and $d\Gamma(H_H)$ commutes with both, the number of particles and W_N . Multiplying (3.36) by $U_{N,t}^*$ we get the first term of (3.33). For the second term of (3.33), we use $W_N^* d\Gamma(H^{(N)}) W_N = H^{(N)}$, and we thus arrive at

$$\mathcal{L}(t) = d\Gamma(H_H) Q_{N,t} + U_{N,t} W_N^* \left(d\Gamma(H^{(N)}) - d\Gamma(H_H^{\phi(t)}) \right) W_N U_{N,t}^*. \quad (3.37)$$

Since the first term commutes with the particle-number operator, it does not contribute to the derivative of $g_N(t; \beta)$ (see (3.34)). We compute the second term, based on the representations (3.28) of $d\Gamma(H^{(N)})$ and $d\Gamma(H_H^{\phi(t)})$ and the properties of the excitation map (3.21). Using that

$$\begin{aligned} U_{N,t} W_N^* a_m^* a_n^* a_q a_p W_N U_{N,t}^* &= U_{N,t} W_N^* a_m^* W_{N-1} U_{N-1,t}^* U_{N-1,t} W_{N-1}^* a_n^* W_{N-2} U_{N-2,t}^* \\ &\quad \times U_{N-2,t} W_{N-2}^* a_q W_{N-1} U_{N-1,t}^* U_{N-1,t} W_{N-1}^* a_p W_N U_{N,t}^* \end{aligned} \quad (3.38)$$

and the notation $\sum_m = \sum_{m \in \mathbb{N}}$ and $\sum_m' = \sum_{m \in \mathbb{N}_+}$, we arrive after a straightforward computation at

$$\begin{aligned}
& U_{N,t} W_N^* \left(d\Gamma(H^{(N)}) - d\Gamma(H_H^{\phi(t)}) \right) W_N U_{N,t}^* = \\
& \frac{1}{2(N-1)} Q_N \left(w_{0000}(N-\mathcal{N})(N-\mathcal{N}-1) + \sum'_{mnpq} w_{mnpq} a_m^* a_n^* a_q a_p \right. \\
& + \sum'_{npq} w_{0npq} \sqrt{N-\mathcal{N}} a_n^* a_q a_p + \sum'_{mpq} w_{m0pq} a_m^* \sqrt{N-\mathcal{N}-1} a_q a_p \\
& + \sum'_{mnq} w_{mn0q} a_m^* a_n^* a_q \sqrt{N-\mathcal{N}} + \sum'_{mnp0} w_{mnp0} a_m^* a_n^* \sqrt{N-\mathcal{N}-1} a_p \\
& + \sum'_{pq} w_{00pq} \sqrt{N-\mathcal{N}} \sqrt{N-\mathcal{N}-1} a_q a_p + \sum'_{nq} w_{0n0q} \sqrt{N-\mathcal{N}} a_n^* a_q \sqrt{N-\mathcal{N}} \\
& + \sum'_{np} w_{0np0} \sqrt{N-\mathcal{N}} a_n^* \sqrt{N-\mathcal{N}-1} a_p + \sum'_{mq} w_{m00q} a_m^* \sqrt{N-\mathcal{N}-1} a_q \sqrt{N-\mathcal{N}} \\
& + \sum'_{mp} w_{m0p0} a_m^* (N-\mathcal{N}-1) a_p + \sum'_{mn} w_{mn00} a_m^* a_n^* \sqrt{N-\mathcal{N}-1} \sqrt{N-\mathcal{N}} \\
& + \sum'_{m} w_{m000} a_m^* (N-\mathcal{N}-1) \sqrt{N-\mathcal{N}} + \sum'_{n} w_{0n00} \sqrt{N-\mathcal{N}} a_n^* \sqrt{N-\mathcal{N}-1} \sqrt{N-\mathcal{N}} \\
& \left. + \sum'_{p} w_{00p0} \sqrt{N-\mathcal{N}} (N-\mathcal{N}-1) a_p + \sum'_{q} w_{000q} \sqrt{N-\mathcal{N}} \sqrt{N-\mathcal{N}-1} a_q \sqrt{N-\mathcal{N}} \right) Q_N \\
& - Q_N \left(\sum'_{mp} w_{m0p0} a_m^* a_p + w_{0000}(N-\mathcal{N}) + \sum'_{m} w_{m000} a_m^* \sqrt{N-\mathcal{N}} + \sum'_{p} w_{00p0} \sqrt{N-\mathcal{N}} a_p \right) Q_N.
\end{aligned} \tag{3.39}$$

We note that we set $e_0 = \phi(t)$, and thus the coefficients w_{k_1, k_2, k_3, k_4} for $k_i \in \mathbb{N}$ depend on time. We can write the r.h.s. as

$$U_{N,t} W_N^* \left(d\Gamma(H^{(N)}) - d\Gamma(H_H) \right) W_N U_{N,t}^* = Q_{N,t} \sum_{\delta=-2}^2 A_{\delta} Q_{N,t}, \tag{3.40}$$

where A_{δ} contains operators that destroy δ particles and $A_{-\delta} = A_{\delta}^*$ contains operators that create δ particles. The terms further simplify by the symmetries under particle permutation of w . In fact, since for the derivative of $g_N(t, \beta)$ the operator A_0 , commuting with the number of particle operator, does not contribute, the only relevant terms are

$$\begin{aligned}
A_1^* &= \frac{1}{(N-1)} \sum'_{mnq} w_{mn0q} a_m^* a_n^* a_q \sqrt{N-\mathcal{N}} - \frac{1}{(N-1)} \sum'_{m} w_{m000} a_m^* \mathcal{N} \sqrt{N-\mathcal{N}}, \\
A_2^* &= \frac{1}{2(N-1)} \sum'_{mn} w_{mn00} a_m^* a_n^* \sqrt{N-\mathcal{N}-1} \frac{\sqrt{N-\mathcal{N}}}{N-1},
\end{aligned} \tag{3.41}$$

and their adjoints operators.

In this step, the Hartree Hamiltonian plays a crucial role: the second term on A_1^* has a contribution of order $N^{3/2}$ coming from the many-body Hamiltonian which cancels when we subtract the contribution from the Hartree Hamiltonian and the final results has the correct scaling $\sqrt{N}$. Thus, we arrive from (3.34) at

$$\partial_t g_N(t, \beta) = -i \langle [\exp(\beta \mathcal{N}), \mathcal{L}(t)] \rangle = \sum_{\delta=1}^2 2 \operatorname{Im} \langle [\exp(\beta \mathcal{N}), A_\delta^*] \rangle. \quad (3.42)$$

As an easy consequence of the commutation relations, we have $\mathcal{N} A_\delta^* = A_\delta^* (\mathcal{N} + \delta)$ and therefore

$$[\exp(\beta \mathcal{N}), A_\delta^*] = 2 \sinh\left(\frac{\beta}{2}\right) \exp\left(\frac{\beta \mathcal{N}}{2}\right) A_\delta^* \exp\left(\frac{\beta \mathcal{N}}{2}\right) \quad (3.43)$$

that enables us to write (3.34) explicitly in terms of creation and annihilation operators as

$$\begin{aligned} \partial_t g(t, \beta) &= 4 \sinh\left(\frac{\beta}{2}\right) \operatorname{Im} \left\langle \sum_{mnq} ' \frac{w_{mn0q}}{N-1} \exp\left(\frac{\beta \mathcal{N}}{2}\right) a_m^* a_n^* a_q \sqrt{N-\mathcal{N}} \exp\left(\frac{\beta \mathcal{N}}{2}\right) \right\rangle \\ &\quad - 4 \sinh\left(\frac{\beta}{2}\right) \operatorname{Im} \left\langle \sum_m ' \frac{w_{m000}}{N-1} \exp\left(\frac{\beta \mathcal{N}}{2}\right) a_m^* \mathcal{N} \sqrt{N-\mathcal{N}} \exp\left(\frac{\beta \mathcal{N}}{2}\right) \right\rangle \\ &\quad + 2 \sinh(\beta) \operatorname{Im} \left\langle \sum_{mn} ' \frac{w_{mn00}}{N-1} \exp\left(\frac{\beta \mathcal{N}}{2}\right) a_m^* a_n^* \sqrt{N-\mathcal{N}-1} \sqrt{N-\mathcal{N}} \exp\left(\frac{\beta \mathcal{N}}{2}\right) \right\rangle. \end{aligned} \quad (3.44)$$

Based on this formula, we derive explicit bounds of the form (3.14) in the next step.

3.2.3 Step 2

While the calculations of the previous section hold for any choice of the interaction potential w , the bounds we prove for all terms of (3.44) will depend on the particular assumptions on w made in Theorem 3.1.1 resp. Theorem 3.1.2. We prove the two cases in separate subsections below.

Mean-field models of type (i)

We start with proving that the estimate (3.14) holds true for any bounded w and with the choice $K := \|w\|$ as in Theorem 3.1.1.

We estimate all terms of (3.44) separately and start with the first. For this we define the following operators by their matrix elements

$$W_{mnpq} = (1 - \delta_{m0}) w_{mnpq} \delta_{p0}, \quad (3.45)$$

$$C_{pqmn} = \frac{1}{N-1} \left\langle \exp \left(\frac{\beta \mathcal{N}}{2} \right) U_{N,t} W_N^* a_m^* a_n^* a_q a_p W_N U_{N,t}^* \exp \left(\frac{\beta \mathcal{N}}{2} \right) \right\rangle, \quad (3.46)$$

for all $m, p \in \mathbb{N}, n, q \in \mathbb{N}_+$. We note that the operator W is bounded, and in particular, its norm is bounded by $\|W\| \leq \|w\|$. The operator C is positive semi-definite. Indeed, for any vector $(v_{mn})_{m \in \mathbb{N}, n \in \mathbb{N}_+}$, we have

$$\begin{aligned} \langle v, Cv \rangle &= \left\langle \exp \left(\frac{\beta \mathcal{N}}{2} \right) U_{N,t} W_N^* \sum_m \sum_n' a_m^* a_n^* \sum_p \sum_q' a_q a_p W_N U_{N,t}^* \exp \left(\frac{\beta \mathcal{N}}{2} \right) \right\rangle \\ &= \left\| \sum_p \sum_q' a_q a_p W_N U_{N,t}^* \exp \left(\frac{\beta \mathcal{N}}{2} \right) \mathcal{U}_N(t, 0) \Xi_N \right\|^2 > 0. \end{aligned} \quad (3.47)$$

Since we will use the inequality $|\text{Tr}(WC)| \leq \|W\| \text{Tr}(C)$, first we compute the trace of C using (3.25) and (3.26)

$$\begin{aligned} \text{Tr}(C) &= \sum_m \sum_n' \frac{1}{N-1} \left\langle \exp \left(\frac{\beta \mathcal{N}}{2} \right) U_{N,t} W_N^* a_m^* a_n^* a_n a_m W_N U_{N,t}^* \exp \left(\frac{\beta \mathcal{N}}{2} \right) \right\rangle \\ &= \frac{1}{N-1} \left\langle U_{N,t} W_N^* \sum_m a_m^* \mathcal{N} a_m W_N U_{N,t}^* \exp(\beta \mathcal{N}) \right\rangle \\ &= \frac{1}{N-1} \left\langle U_{N,t} W_N^* \left(\sum_m' a_m^* a_m (\mathcal{N}_+ - 1) + a_0^* a_0 \mathcal{N}_+ \right) W_N U_{N,t}^* \exp(\beta \mathcal{N}) \right\rangle \quad (3.48) \\ &= \frac{1}{N-1} \langle U_{N,t} W_N^* \mathcal{N}_+ (\mathcal{N} - 1) W_N U_{N,t}^* \exp(\beta \mathcal{N}) \rangle \\ &= \frac{1}{N-1} \langle \mathcal{N}(\mathcal{N} - 1) \exp(\beta \mathcal{N}) \rangle \\ &= \partial_\beta g_N(t, \beta), \end{aligned}$$

where in the last step we identified $\partial_\beta g_N(t, \beta) = \langle \mathcal{N} \exp(\beta \mathcal{N}) \rangle$. Using the operators W and C defined in (3.45) resp. (3.46), the first term in equation (3.44) can be bounded by

$$\begin{aligned} &4 \sinh \left(\frac{\beta}{2} \right) \left| \left\langle \sum_{mnq}' \frac{w_{mn0q}}{N-1} \exp \left(\frac{\beta \mathcal{N}}{2} \right) a_m^* a_n^* a_q \sqrt{N - \mathcal{N}_+} \exp \left(\frac{\beta \mathcal{N}}{2} \right) \right\rangle \right| \\ &= 4 \sinh \left(\frac{\beta}{2} \right) \left| \left\langle \sum_{mp} \sum_{nq}' (1 - \delta_{m0}) \frac{w_{mnpq}}{N-1} \delta_{p0} \exp \left(\frac{\beta \mathcal{N}}{2} \right) a_m^* a_n^* a_q \sqrt{N - \mathcal{N}_+} \exp \left(\frac{\beta \mathcal{N}}{2} \right) \right\rangle \right| \\ &= 4 \sinh \left(\frac{\beta}{2} \right) |\text{Tr}(WC)| \\ &\leq 4 \sinh \left(\frac{\beta}{2} \right) \|w\| \partial_\beta g_N(t, \beta). \end{aligned} \quad (3.49)$$

For the second term of equation (3.44), we define the following operators by their matrix elements

$$\tilde{W}_{mp} = (1 - \delta_{m0}) w_{m0p0} \delta_{p0}, \quad \forall m, p \in \mathbb{N}, \quad (3.50)$$

$$\tilde{C}_{pm} = \frac{1}{N-1} \left\langle \exp \left(\frac{\beta \mathcal{N}}{2} \right) U_N W_N^* a_m^* \mathcal{N}_+ a_p W_N U_N^* \exp \left(\frac{\beta \mathcal{N}}{2} \right) \right\rangle, \quad \forall m, p \in \mathbb{N}. \quad (3.51)$$

We note that $\tilde{W}$ is bounded with norm $\|\tilde{W}\| \leq \|w\|$ and the operator $\tilde{C}$ is positive with trace

$$\begin{aligned} \text{Tr}(\tilde{C}) &= \frac{1}{N-1} \sum_m \left\langle \exp \left(\frac{\beta \mathcal{N}}{2} \right) U_N W_N^* a_m^* \mathcal{N}_+ a_m W_N U_N^* \exp \left(\frac{\beta \mathcal{N}}{2} \right) \right\rangle \\ &= \frac{1}{N-1} \left\langle U_N W_N^* \left(\sum_m' a_m^* a_m (\mathcal{N}_+ - 1) + a_0^* a_0 \mathcal{N}_+ \right) W_N U_N^* \exp(\beta \mathcal{N}) \right\rangle \\ &= \frac{1}{N-1} \langle U_N W_N^* (\mathcal{N} - 1) \mathcal{N}_+ W_N U_N^* \exp(\beta \mathcal{N}) \rangle \\ &= \frac{1}{N-1} \langle (N-1) \mathcal{N} \exp(\beta \mathcal{N}) \rangle \\ &= \partial_\beta g_N(t, \beta). \end{aligned} \quad (3.52)$$

With these definitions, we estimate the second term of (3.44) by

$$\begin{aligned} &4 \sinh \left(\frac{\beta}{2} \right) \left| \left\langle \sum_m' \frac{w_{m000}}{N-1} \exp \left(\frac{\beta \mathcal{N}}{2} \right) a_m^* \mathcal{N} \sqrt{N - \mathcal{N}} \exp \left(\frac{\beta \mathcal{N}}{2} \right) \right\rangle \right| \\ &= 4 \sinh \left(\frac{\beta}{2} \right) \left| \left\langle \sum_{mp} (1 - \delta_{m0}) \frac{w_{m0p0}}{N-1} \delta_{p0} \exp \left(\frac{\beta \mathcal{N}}{2} \right) U_N W_N^* a_m^* \mathcal{N}_+ a_p W_N U_N^* \exp \left(\frac{\beta \mathcal{N}}{2} \right) \right\rangle \right| \\ &= 4 \sinh \left(\frac{\beta}{2} \right) |\text{Tr}(\tilde{W} \tilde{C})| \\ &\leq 4 \sinh \left(\frac{\beta}{2} \right) \|w\| \partial_\beta g_N(t, \beta). \end{aligned} \quad (3.53)$$

For the third term of equation (3.44), we will use a different bound: we define the following vectors with entries

$$v_{mn} = w_{mn00} \quad \forall m, n \in \mathbb{N}_+, \quad (3.54)$$

$$u_{mn} = \frac{1}{N-1} \left\langle \exp \left(\frac{\beta \mathcal{N}}{2} \right) a_m^* a_n^* \sqrt{N - \mathcal{N} - 1} \sqrt{N - \mathcal{N}} \exp \left(\frac{\beta \mathcal{N}}{2} \right) \right\rangle \quad \forall m, n \in \mathbb{N}_+. \quad (3.55)$$

Since w is bounded, we have

$$\sqrt{\sum_{mn} |w_{mnpq}|^2} \leq \|w\| \quad \forall p, q \in \mathbb{N}, \quad (3.56)$$

and furthermore

$$\|v\|^2 = \sum'_{mn} |w_{mn00}|^2 \leq \|w\|^2. \quad (3.57)$$

To compute the norm of the vector u , we artificially add $1 = (\mathcal{N} + 1)^{-1/2}(\mathcal{N} + 1)^{1/2}$ and estimate with the Cauchy–Schwarz inequality

$$\begin{aligned} \|u\|^2 &= \frac{1}{(N-1)^2} \sum'_{mn} \left| \left\langle \exp\left(\frac{\beta\mathcal{N}}{2}\right) a_m^* a_n^* \frac{(\mathcal{N}+1)^{1/2}}{(\mathcal{N}+1)^{1/2}} \sqrt{N-\mathcal{N}-1} \sqrt{N-\mathcal{N}} \exp\left(\frac{\beta\mathcal{N}}{2}\right) \right\rangle \right|^2 \\ &\leq \frac{1}{(N-1)^2} \sum'_{mn} \left\langle \exp\left(\frac{\beta\mathcal{N}}{2}\right) a_m^* a_n^* (\mathcal{N}+1)^{-1} a_n a_m \exp\left(\frac{\beta\mathcal{N}}{2}\right) \right\rangle \\ &\quad \times \langle (\mathcal{N}+1)(N-\mathcal{N}-1)(N-\mathcal{N}) \exp(\beta\mathcal{N}) \rangle \\ &\leq \left\langle \sum'_{mn} a_m^* a_n^* a_n a_m (\mathcal{N}-1)^{-1} \exp(\beta\mathcal{N}) \right\rangle \left\langle (\mathcal{N}+1) \frac{(N-\mathcal{N}-1)(N-\mathcal{N})}{(N-1)^2} \exp(\beta\mathcal{N}) \right\rangle \\ &\leq \langle \mathcal{N} \exp(\beta\mathcal{N}) \rangle \langle (\mathcal{N}+1) \exp(\beta\mathcal{N}) \rangle \\ &\leq \langle (\mathcal{N}+1) \exp(\beta\mathcal{N}) \rangle^2. \end{aligned} \quad (3.58)$$

With these notations and bounds, we get for the third term of (3.44)

$$\begin{aligned} &2 \sinh(\beta) \left| \left\langle \sum'_{mn} \frac{w_{mn00}}{N-1} \exp\left(\frac{\beta\mathcal{N}}{2}\right) a_m^* a_n^* \sqrt{N-\mathcal{N}-1} \sqrt{N-\mathcal{N}} \exp\left(\frac{\beta\mathcal{N}}{2}\right) \right\rangle \right| \\ &= 2 \sinh(\beta) | \langle v, u \rangle | \\ &\leq 2 \sinh(\beta) \|v\| \|u\| \\ &\leq 2 \sinh(\beta) \|w\| (g_N(t, \beta) + \partial_\beta g_N(t, \beta)). \end{aligned} \quad (3.59)$$

Summing up the three bounds (3.49), (3.53) and (3.59), we get as a final bound for (3.44)

$$\partial_t g_N(t, \beta) \leq \left(8 \|w\| \sinh\left(\frac{\beta}{2}\right) + 2 \|w\| \sinh(\beta) \right) \partial_\beta g_N(t, \beta) + 2 \sinh(\beta) \|w\| g_N(t, \beta), \quad (3.60)$$

that proves the claim.

Mean-field models of type (ii)

Now we will prove the claim (3.14) under the assumptions of Theorem 3.1.2. We start by rewriting (3.44) using that in this case w is a multiplication operator. Since the interaction is given by a multiplication operator of the form $w(x; y) = V(x - y)$, we have

$$w_{mnpq} = \int dx dy \bar{e}_m(x) \bar{e}_n(y) V(x - y) e_p(x) e_q(y). \quad (3.61)$$

We observe that, formally, since the expectation value in (3.44) is evaluated in wavefunctions on the orthogonal Fock space $\mathcal{F}_{\perp \phi(t)}^{\leq N}$, we can replace $\sum'$ by $\sum$ in all three terms of (3.44). Therefore, using the identity $\sum_n \bar{e}_n(x) e_n(y) = \delta(x - y)$, the linearity $\sum_n \alpha_n a_n^* = a^*(\sum_n \alpha_n e_n)$, and

$$\sum_n \bar{e}_n(x) a_n^* = a^*(\sum_n e_n(x) e_n) = a^*(\delta(x - \cdot)) =: a_x^*. \quad (3.62)$$

we can write (3.44) as

$$\begin{aligned} \partial_t g(t, \beta) &= 4 \sinh\left(\frac{\beta}{2}\right) \operatorname{Im} \left\langle \int dx dy \frac{V(x - y)}{N - 1} \phi(t, x) \exp\left(\frac{\beta \mathcal{N}}{2}\right) a_x^* a_y^* a_y \sqrt{N - \mathcal{N}} \exp\left(\frac{\beta \mathcal{N}}{2}\right) \right\rangle \\ &\quad - 4 \sinh\left(\frac{\beta}{2}\right) \operatorname{Im} \left\langle \int dx dy \frac{V(x - y)}{N - 1} \bar{\phi}(t, y) \phi(t, x) \phi(t, y) \exp\left(\frac{\beta \mathcal{N}}{2}\right) a_x^* \mathcal{N} \sqrt{N - \mathcal{N}} \exp\left(\frac{\beta \mathcal{N}}{2}\right) \right\rangle \\ &\quad + 2 \sinh(\beta) \operatorname{Im} \left\langle \int dx dy \frac{V(x - y)}{N - 1} \phi(t, x) \phi(t, y) \exp\left(\frac{\beta \mathcal{N}}{2}\right) a_x^* a_y^* \sqrt{N - \mathcal{N} - 1} \sqrt{N - \mathcal{N}} \exp\left(\frac{\beta \mathcal{N}}{2}\right) \right\rangle. \end{aligned} \quad (3.63)$$

To bound each of these terms we use that the creation and annihilation operators are bounded in terms of the number of particles operator by

$$\|a^*(f)\Psi\| \leq \|f\|_{L^2} \sqrt{\mathcal{N} + 1} \|\Psi\|, \quad \|a(f)\Psi\| \leq \|f\|_{L^2} \sqrt{\mathcal{N}} \|\Psi\| \quad \forall \Psi \in \mathcal{F}, \quad (3.64)$$

valid for all $\Psi \in \mathcal{F}$. On the orthogonal Fock space $\mathcal{F}_{\perp \phi(t)}^{\leq N}$ we furthermore have

$$\|\mathcal{N}\Psi\| \leq N \|\Psi\| \quad \forall \Psi \in \mathcal{F}^{\leq N}. \quad (3.65)$$

Moreover, we use that $\|\phi(t)\|_{L^2} = 1 \forall t$ and the constant $\mathbb{V}$ defined in (3.8) can be written as

$$\mathbb{V} = \sup_x \|V(x - \cdot) \phi(t)\|_{L^2}. \quad (3.66)$$

Now we bound each term in (3.63) separately using that $\int f(x) a_x^* dx = a^*(f)$, the Cauchy-Schwarz inequality and the inequalities (3.64), (3.65).

We start with the first term that we estimate with

$$\begin{aligned}
& \left| 4 \sinh \left(\frac{\beta}{2} \right) \operatorname{Im} \left\langle \int dx dy \frac{V(x-y)}{N-1} \phi(t, x) \exp \left(\frac{\beta \mathcal{N}}{2} \right) a_x^* a_y^* a_y \sqrt{N-\mathcal{N}} \exp \left(\frac{\beta \mathcal{N}}{2} \right) \right\rangle \right| \\
& \leq \frac{4}{N-1} \sinh \left(\frac{\beta}{2} \right) \int dy \left| \left\langle \exp \left(\frac{\beta \mathcal{N}}{2} \right) a_y^* a^*(V(y-\cdot)\phi(t)) \sqrt{N-\mathcal{N}-1} a_y \exp \left(\frac{\beta \mathcal{N}}{2} \right) \right\rangle \right| \\
& \leq \frac{4}{N-1} \sinh \left(\frac{\beta}{2} \right) \int dy \|a(V(y-\cdot)\phi(t)) a_y \exp \left(\frac{\beta \mathcal{N}}{2} \right) \mathcal{U}_N(t, 0) \Xi_N\| \\
& \quad \times \|\sqrt{N-\mathcal{N}-1} a_y \exp \left(\frac{\beta \mathcal{N}}{2} \right) \mathcal{U}_N(t, 0) \Xi_N\| \\
& \leq \frac{4}{N-1} \sinh \left(\frac{\beta}{2} \right) \int dy \mathbb{V}(N-1) \|a_y \exp \left(\frac{\beta \mathcal{N}}{2} \right) \mathcal{U}_N(t, 0) \Xi_N\|^2 \\
& \leq 4 \mathbb{V} \sinh \left(\frac{\beta}{2} \right) \langle \mathcal{N} \exp(\beta \mathcal{N}) \rangle = 4 \mathbb{V} \sinh \left(\frac{\beta}{2} \right) \partial_{\beta} g_N(t, \beta).
\end{aligned} \tag{3.67}$$

With similar ideas, we bound the second term by

$$\begin{aligned}
& \left| 4 \sinh \left(\frac{\beta}{2} \right) \operatorname{Im} \left\langle \int dx dy \frac{V(x-y)}{N-1} \bar{\phi}(t, y) \phi(t, x) \phi(t, y) \exp \left(\frac{\beta \mathcal{N}}{2} \right) a_x^* \mathcal{N} \sqrt{N-\mathcal{N}} \exp \left(\frac{\beta \mathcal{N}}{2} \right) \right\rangle \right| \\
& \leq \frac{4}{N-1} \sinh \left(\frac{\beta}{2} \right) \int dy |\phi(t, y)|^2 \left| \left\langle \exp \left(\frac{\beta \mathcal{N}}{2} \right) a^*(V(y-\cdot)\phi(t)) \mathcal{N} \sqrt{N-\mathcal{N}} \exp \left(\frac{\beta \mathcal{N}}{2} \right) \right\rangle \right| \\
& \leq \frac{4}{N-1} \sinh \left(\frac{\beta}{2} \right) \int dy |\phi(t, y)|^2 \|\sqrt{\mathcal{N}} a(V(y-\cdot)\phi(t)) \exp \left(\frac{\beta \mathcal{N}}{2} \right) \mathcal{U}_N(t, 0) \Xi_N\| \\
& \quad \times \|\sqrt{\mathcal{N}} \sqrt{N-\mathcal{N}} \exp \left(\frac{\beta \mathcal{N}}{2} \right) \mathcal{U}_N(t, 0) \Xi_N\| \\
& \leq \frac{4}{N-1} \sinh \left(\frac{\beta}{2} \right) \mathbb{V} N \|\sqrt{\mathcal{N}} \exp \left(\frac{\beta \mathcal{N}}{2} \right) \mathcal{U}_N(t, 0) \Xi_N\|^2 \\
& \leq 4 \mathbb{V} \frac{N}{N-1} \sinh \left(\frac{\beta}{2} \right) \langle \mathcal{N} \exp(\beta \mathcal{N}) \rangle \\
& \leq 4 \mathbb{V} (1 + \epsilon) \sinh \left(\frac{\beta}{2} \right) \partial_{\beta} g_N(t, \beta).
\end{aligned} \tag{3.68}$$

We remark that the last step holds true for any $\epsilon > 1/(N-1)$. Lastly, we bound the third

term by

$$\begin{aligned}
& \left| 2 \sinh(\beta) \operatorname{Im} \left\langle \int dx dy \frac{V(x-y)}{N-1} \phi(t, x) \phi(t, y) \exp\left(\frac{\beta \mathcal{N}}{2}\right) a_x^* a_y^* \sqrt{N-\mathcal{N}-1} \sqrt{N-\mathcal{N}} \exp\left(\frac{\beta \mathcal{N}}{2}\right) \right\rangle \right| \\
& \leq \frac{2}{N-1} \sinh(\beta) \int dx \left| \phi(t, x) \left\langle \exp\left(\frac{\beta \mathcal{N}}{2}\right) a_x^* \sqrt{N-\mathcal{N}} a^*(V(x-\cdot)\phi(t)) \sqrt{N-\mathcal{N}} \exp\left(\frac{\beta \mathcal{N}}{2}\right) \right\rangle \right| \\
& \leq \frac{2}{N-1} \sinh(\beta) \int dx |\phi(t, x)| \|\sqrt{N-\mathcal{N}} a_x \exp\left(\frac{\beta \mathcal{N}}{2}\right) \mathcal{U}_N(t, 0) \Xi_N\| \\
& \quad \times \|a^*(V(x-\cdot)\phi(t)) \sqrt{N-\mathcal{N}} \exp\left(\frac{\beta \mathcal{N}}{2}\right) \mathcal{U}_N(t, 0) \Xi_N\| \\
& \leq \frac{2}{N-1} \sinh(\beta) \|\sqrt{N-\mathcal{N}} a(\phi(t)) \exp\left(\frac{\beta \mathcal{N}}{2}\right) \mathcal{U}_N(t, 0) \Xi_N\| \\
& \quad \times \mathbb{V} \|\sqrt{\mathcal{N}+1} \sqrt{N-\mathcal{N}} \exp\left(\frac{\beta \mathcal{N}}{2}\right) \mathcal{U}_N(t, 0) \Xi_N\| \\
& \leq 2\mathbb{V} \frac{N}{N-1} \sinh(\beta) \|\sqrt{\mathcal{N}+1} \exp\left(\frac{\beta \mathcal{N}}{2}\right) \mathcal{U}_N(t, 0) \Xi_N\|^2 \\
& \leq 2\mathbb{V}(1+\epsilon) \sinh(\beta) (\partial_\beta g_N(t, \beta) + g_N(t, \beta)).
\end{aligned} \tag{3.69}$$

To simplify the notation we multiply the bound on (3.67) by $1+\epsilon$. Furthermore, since $N \geq 2$, we fix $\epsilon = 1$. Summing up the three bounds (3.67), (3.68) and (3.69), we arrive at

$$\partial_t g_N(t, \beta) \leq \left(16\mathbb{V} \sinh \frac{\beta}{2} + 4\mathbb{V} \sinh \beta \right) \partial_\beta g_N(t, \beta) + 4 \sinh \beta \mathbb{V} g_N(t, \beta), \tag{3.70}$$

that proves the desired claim.

3.2.4 Step 3

In the last step, we prove the final estimate of Theorem 3.1.2 resp. Theorem 3.1.1 from (3.14) based on a Gronwall type argument. Since this argument does not depend on the choice of K in the estimate (3.14), this part of the proof is again the same for both Theorems.

To simplify the calculations, we first bound

$$8K \sinh \frac{\beta}{2} + 2K \sinh \beta \leq 6K \sinh \beta. \tag{3.71}$$

and write (3.14) as

$$\frac{1}{2K \sinh \beta} \partial_t g_N(t, \beta) + 3 \partial_\beta g_N(t, \beta) \leq g_N(t, \beta). \tag{3.72}$$

In particular note that all coefficients in front of (derivatives of) $g_N(t, \beta)$ are independent of N . However, before we can apply Gronwall's lemma, we need to perform a suitable change of variables $x = X(t, \beta)$ and $y = Y(t, \beta)$ such that the inequality takes the form

$$\partial_y g_N \leq g_N. \quad (3.73)$$

In fact, from (3.73), we then arrive for fixed x from Gronwall's inequality at

$$g_N(x, y) \leq g_N(x, y_0) e^{y-y_0} \quad (3.74)$$

for arbitrary $y_0 \in \mathbb{R}$. We define y_0 through the inverse change of variables $t = T(x, y)$ and $\beta = B(x, y)$ such that it realizes the initial conditions $g_N(t = 0, \beta) \leq C_\beta$, i.e. we define y_0 through

$$T(X(t, \beta), y_0) = 0, \quad (3.75)$$

such that $g_N(x, y_0) \leq C_\beta$. Thus, the change of variables (X, Y) , solves

$$\frac{1}{2K \sinh \beta} \partial_t X - 3 \partial_\beta X = 0, \quad \text{and} \quad \frac{1}{2K \sinh \beta} \partial_t Y - 3 \partial_\beta Y = 1. \quad (3.76)$$

The functions

$$X(t, \beta) = 6Kt - 2 \operatorname{artanh}(e^{-\beta}), \quad \text{and} \quad Y(t, \beta) = 6Kt - 2 \operatorname{artanh}(e^{-\beta}) - \frac{\beta}{3} \quad (3.77)$$

solve the equations and any other solution is a reparameterization of this variables and will therefore not change the result. The inverse change of variables is given by

$$T(x, y) = \frac{1}{6K} \left(x + 2 \operatorname{artanh} \left(e^{-3(x-y)} \right) \right), \quad \text{and} \quad B(x, y) = 3(x - y). \quad (3.78)$$

Since $\beta \geq 0$ by assumption, we find $x - y \geq 0$. From (3.75) we finally get

$$y_0(t, \beta) = 6Kt - 2 \operatorname{artanh}(e^{-\beta}) + \frac{1}{3} \ln \left(\tanh \left(\operatorname{artanh}(e^{-\beta}) - 3Kt \right) \right) \quad (3.79)$$

for all

$$0 \leq \beta < \beta_c(t) := -\ln \tanh(3Kt), \quad (3.80)$$

that ensures the argument of the logarithm is positive. Thus the initial condition $g_N(x, y_0) \leq C_\beta$ is realized only for $\beta < \beta_c(t)$. With the choices (3.77) and (3.79) in (3.74) we finally arrive at

$$g_N(t, \beta) \leq C_\beta \left(\frac{1 - \tanh(3Kt)e^{-\beta}}{1 - \tanh(3Kt)e^\beta} \right)^{\frac{1}{3}}. \quad (3.81)$$

3.3 Conclusions

In this chapter, we have analyzed the persistence of condensation for bosonic many-body systems evolving under mean-field dynamics, with a particular focus on the quantitative control of the number of excitations above the condensate. Starting from initial data exhibiting an exponential concentration of the number of excitations, we proved that this property is preserved for all finite times: the probability of finding n particles outside the condensate decays exponentially in n , uniformly in the total particle number N .

Our results apply to two broad and physically relevant classes of models: systems with arbitrary bounded two-body interactions, encompassing a wide range of finite-dimensional and effective mean-field models, and continuum systems with unbounded interaction potentials satisfying the operator inequality $V^2 \leq D(1 - \Delta)$, including Coulomb-type interactions. In both settings, the exponential control of the number of excitations significantly sharpens previously available bounds, which were limited to polynomial decay derived from uniform estimates on finitely many moments of the excitation number operator.

From a physical perspective, the exponential concentration of the number of excitations provides a refined description of the many-body state beyond the leading-order Hartree dynamics. This type of control is particularly relevant in situations where rare but large fluctuations may play a role, for instance in the study of correlation functions or in the justification of effective theories for excitations.

On the mathematical side, our results contribute to the growing body of work aimed at a detailed understanding of fluctuations in bosonic mean-field limits. They suggest that, at least for finite times, the excitation structure of the many-body wavefunction is considerably more rigid than what moment bounds alone can capture. It remains an open question to understand if the exponential condensation holds true also in the Gross-Pitaevskii scaling regime.

Chapter 4

Quantum linear system solver

In this chapter, we analyze the HHL algorithm presented in section 1.4 and its variant. Since the *HHL variant* assumes a known upper bound on the condition number, we extend the analysis to the case where such a bound is unknown, showing that the error fails to converge to zero even for a large number of qubits. We then propose a modification of the *HHL variant* that preserves its simplicity, thus remaining experimentally feasible, and restores the convergence of the final output error to zero for a large number of qubits in the second register.

Our analysis then clarifies the theoretical structure of quantum algorithms for linear problems, and can be generalized to algorithms exploiting recently developed alternatives to the quantum phase estimation [160–166]. We also carefully consider the complexity of the algorithm in the light of recent results on simulations of unitaries [34, 77, 78, 80–85] used in the quantum phase estimation step.

In section 4.1, we analyze the convergence of the algorithm’s outcome towards the exact solution and emphasize the difference between the original and the variant algorithms. The *improved HHL variant* is derived in section 4.2. We compare the complexity of the above algorithms in section 4.3. Sections 4.4 and 4.5 are devoted, respectively, to numerical simulations of the *HHL variant* and the improved algorithm, and to the relaxation of a technical assumption (the positivity of A). Long and technical calculations are provided in Appendix A.

4.1 Error analysis

In this section, we discuss how close the output states of the *HHL algorithm* and of its variant are to the ideal solution of the linear problem (1.43). The ideal output of the

algorithm is the embedding of the vector $\mathbf{x}$ (1.45) in the r -register as follows

$$|x\rangle = |1\rangle_a |0\rangle_c \frac{C}{\sqrt{p}} \sum_{j=0}^{2^n-1} \frac{\beta_j}{\lambda_j} |u_j\rangle_r, \quad (4.1)$$

where we wrote the normalization constant as $C/\sqrt{p}$ in order to make the expression more similar to (1.56), and the normalization of the state (4.1) entails

$$p = \sum_{j=0}^{2^n-1} \left(\frac{C |\beta_j|}{\lambda_j} \right)^2. \quad (4.2)$$

Since $\sin(\theta(k)) = Ct_0/(2\pi k)$ is the amplitude of the component $|1\rangle_a$ in the state (1.51), the constant C must satisfy $C \leq 2\pi k/t_0$ for all $k \geq k_{\min}$. We then choose the largest of the allowed values $C = 2\pi k_{\min}/t_0 \simeq 1/(2\kappa')$ that maximizes the ideal and the actual probability of measuring $|1\rangle_a$, respectively p and p_0 .

Before proceeding with our analysis, we stress that the precision of the eigenvalue estimation in the phase estimation subroutine is improved by increasing t_0 . The reason is that the eigenvalues λ_j are amplified and can be better distinguished. On the other hand, the phase estimation cannot differentiate phases modulo 2π , and if $\lambda_j t_0/T > 2\pi$ the protocol fails. Therefore, under the assumption $0 < \lambda_j \leq 1$ for all j , we can take t_0 proportional to T , $t_0 = tT$ for some $0 < t < 2\pi$. Given $\lambda_{\min} := \min_j \{\lambda_j\}$, this scaling implies $p = \mathcal{O}(C/\lambda_{\min})^2 = \mathcal{O}((2\pi k_{\min})^2/(\lambda_{\min} t T)^2) = \mathcal{O}(\kappa/\kappa')^2$.

The states $|x\rangle$ and $|x_0\rangle$ are close to each other if their squared overlap, also called fidelity $|\langle x|x_0\rangle|^2$, is close to 1. We then consider the so-called *infidelity* $1 - |\langle x|x_0\rangle|^2$ as a measure of the deviation of the output state $|x_0\rangle$ from the ideal state $|x\rangle$. Indeed, the square root of the infidelity satisfies the properties of a distance between pure states [167, 168],

$$d(|x\rangle, |x_0\rangle) := \sqrt{1 - |\langle x|x_0\rangle|^2}, \quad (4.3)$$

and we shall use $d(|x\rangle, |x_0\rangle)$ to quantify the error of the algorithm.

In the original article [33], they show an upper bound for the difference between the ideal and the actual output of the *HHL algorithm*, which implies

$$d(|x\rangle, |x_0^{\text{HHL}}\rangle) \leq \mathcal{O}(\kappa/T). \quad (4.4)$$

The main result of this section is given by the following theorem, where we show a lower bound for the difference between the ideal and the actual output of the *HHL variant*.

Theorem 4.1.1 (Lower bound on the convergence of the *HHL variant*). *Given the ideal output of the HHL algorithm (4.1) and the output state of the HHL variant (1.56), with coefficients $\alpha_{k|j}^{\text{var}}$ given by (1.54), the distance between these states is lower bounded by*

$$d(|x\rangle, |x_0^{\text{var}}\rangle) \geq \Omega\left(\frac{\kappa'}{T} + \sqrt{\frac{\kappa}{T} \ln \frac{T}{\kappa}}\right). \quad (4.5)$$

The big omega notation, $f \geq \Omega(g)$, in complexity theory means that there is some constant $k > 0$ such that $f(T) \geq k \cdot g(T)$ for large enough values of T .

Proof. We start by computing the overlap $\langle x | x_0^{\text{var}} \rangle$. A straightforward computation shows that

$$\frac{1}{\sqrt{T}} \sum_{\sigma=0}^{T-1} e^{i\frac{\sigma}{T}(2\pi k - \lambda_j t T)} \langle 0 | (C^{\text{var}})^{-1} | \sigma \rangle = \alpha_{k|j}^{\text{var}}. \quad (4.6)$$

Then, we can compute the overlap between the ideal and the actual outputs,

$$\begin{aligned} \langle x | x_0^{\text{var}} \rangle &= \frac{C^2}{\sqrt{p} p_0} \sum_{j=0}^{2^n-1} \frac{|\beta_j|^2}{\lambda_j} \sum_{k=k_{\min}}^{T-1} |\alpha_{k|j}^{\text{var}}|^2 \frac{t T}{2\pi k} \\ &= \frac{\sum_{j=0}^{2^n-1} \frac{|\beta_j|^2}{\lambda_j} \sum_{k=k_{\min}}^{T-1} |\alpha_{k|j}^{\text{var}}|^2 \frac{t T}{2\pi k}}{\sqrt{\sum_{l=0}^{2^n-1} \frac{|\beta_l|^2}{\lambda_l^2} \sum_{j=0}^{2^n-1} |\beta_j|^2 \sum_{k=k_{\min}}^{T-1} \left(|\alpha_{k|j}^{\text{var}}|^2 \frac{t T}{2\pi k}\right)^2}}. \end{aligned} \quad (4.7)$$

Moreover, the following quantities

$$\epsilon_{1,j}^{\text{var}} := \lambda_j \left(\sum_{k=k_{\min}}^{T-1} |\alpha_{k|j}^{\text{var}}|^2 \frac{t T}{2\pi k} - \frac{1}{\lambda_j} \right), \quad (4.8)$$

$$\epsilon_{2,j}^{\text{var}} := \lambda_j^2 \left(\sum_{k=k_{\min}}^{T-1} |\alpha_{k|j}^{\text{var}}|^2 \left(\frac{t T}{2\pi k} \right)^2 - \frac{1}{\lambda_j^2} \right), \quad (4.9)$$

are useful to study the convergence of the distance $d(|x\rangle, |x_0^{\text{var}}\rangle)$ for large dimension of the clock Hilbert space, $T = 2^{n_c}$,

$$d(|x\rangle, |x_0^{\text{var}}\rangle) = \sqrt{\frac{\sum_{j,l=0}^{2^n-1} \frac{|\beta_j|^2 |\beta_l|^2}{\lambda_j^2 \lambda_l^2} (\epsilon_{2,j}^{\text{var}} - \epsilon_{1,j}^{\text{var}} - \epsilon_{1,l}^{\text{var}} - \epsilon_{1,j}^{\text{var}} \epsilon_{1,l}^{\text{var}})}{\sum_{j,l=0}^{2^n-1} \frac{|\beta_j|^2 |\beta_l|^2}{\lambda_j^2 \lambda_l^2} (1 + \epsilon_{2,j}^{\text{var}})}}. \quad (4.10)$$

Given a fixed j , we can interpret $\epsilon_{1,j}^{\text{var}}$ as a measure of how well the algorithm approximates the inverse eigenvalue $1/\lambda_j$ by the average of $tT/(2\pi k)$ over the distribution $|\alpha_{k|j}^{\text{var}}|^2$.

The following lemma shows a lower bound for this quantity. We postpone the proof to section A.2.

Lemma 4.1.2 (Approximation of the inverse eigenvalues). *Fix some $j = 0, \dots, 2^n - 1$, the error on the approximation of the HHL variant of the inverse of the eigenvalue λ_j , given by (4.8), has the following asymptotic behavior for large T :*

$$|\epsilon_{1,j}^{\text{var}}| \leq \mathcal{O}\left(\frac{\ln(\lambda_j t T)}{\lambda_j t T}\right). \quad (4.11)$$

At the same time, $\epsilon_{2,j}^{\text{var}}$ measures how well the algorithm approximates the inverse squared eigenvalue $1/\lambda_j^2$ by the average of $(tT/2\pi k)^2$ over the distribution given by $|\alpha_{k|j}^{\text{var}}|^2$. The following lemma shows that the lower and upper bounds depend not only on T , but also on κ' . We postpone the proof to section A.3.

Lemma 4.1.3 (Approximation of the inverse squared eigenvalues). *Fix some $j = 0, \dots, 2^n - 1$, the error on the approximation of the HHL variant of the inverse square of the eigenvalue λ_j , given by (4.9), has the following asymptotic behavior for large T :*

$$\Omega\left(\left(\frac{\kappa'}{T}\right)^2 + \frac{\ln(\lambda_j t T)}{\lambda_j t T}\right) \leq |\epsilon_{2,j}^{\text{var}}| \leq \mathcal{O}\left(\frac{\kappa'}{tT} + \frac{\ln(\lambda_j t T)}{\lambda_j t T}\right). \quad (4.12)$$

To establish the lower bound (4.5), we evaluate the fraction inside the square root of (4.10) by simultaneously lower-bounding its numerator and upper-bounding its denominator. To minimize the numerator, we replace $\epsilon_{2,j}^{\text{var}}$ with its asymptotic lower bound from Lemma 4.1.3 and subtract the absolute upper bounds of the first-order errors $|\epsilon_{1,j}^{\text{var}}|$ and $|\epsilon_{1,l}^{\text{var}}|$ provided by Lemma 4.1.2. Since the product $\epsilon_{1,j}^{\text{var}} \epsilon_{1,l}^{\text{var}}$ is of strictly higher order, its contribution is absorbed into the existing asymptotic error scaling. For the denominator, in the limit of large clock dimension $T = 2^{n_c}$, Lemma 4.1.3 allows the denominator to be upper-bounded by $\sum_{j,l} \frac{|\beta_j|^2 |\beta_l|^2}{\lambda_j^2 \lambda_l^2} (1 + \mathcal{O}(1))$. Consequently, the distance $d(|x\rangle, |x_0^{\text{var}}\rangle)$ is bounded below by the square root of the weighted average of these asymptotic terms. The worst-case global scaling is dominated by the smallest eigenvalue in the spectrum. Assuming the matrix A is normalized such that its maximum eigenvalue is a strictly positive constant independent of T , i.e., $\lambda_{\max} = \mathcal{O}(1)$, the minimum eigenvalue scales exactly as the inverse of the condition number, $\lambda_{\min} = \mathcal{O}(\kappa^{-1})$. Evaluating the bounds at $\lambda_{\min}$ yields:

$$d(|x\rangle, |x_0^{\text{var}}\rangle) \geq \sqrt{\Omega\left(\left(\frac{\kappa'}{T}\right)^2\right) + \Omega\left(\frac{\kappa}{T} \ln \frac{T}{\kappa}\right)}. \quad (4.13)$$

By the asymptotic property for non-negative quantities, $\sqrt{\Omega(x) + \Omega(y)} = \Omega(\sqrt{x}) + \Omega(\sqrt{y})$, we extract the dominant terms from the square root. This yields the desired combined lower bound (4.5), which concludes the proof. $\square$

Theorem 4.1.1 implies that the *HHL variant* is accurate when both the condition number κ and its computable bound κ' are much smaller than T , resulting in $k_{\min} = \lfloor tT/(4\pi\kappa') \rfloor \gg 1$. The *HHL variant* is then not accurate if the bound κ' is as large as T ($k_{\min} \sim 1$) even when $\kappa \ll T$. This implies that the implementation of the *HHL variant* requires having an estimate of the condition number, otherwise the convergence is not guaranteed.

The convergence problem of the *HHL variant* can be understood from equation (1.56). Recalling that $C^{\text{var}} = H^{\otimes n_c}$ in this case, the coefficients of the states with fixed $|\gamma\rangle_c$ are proportional to

$$\frac{\alpha_{k|j}^{\text{var}}}{T} \sum_{\sigma=0}^{T-1} e^{i\frac{\sigma}{T}(2\pi k - \lambda_j t_0) + i\pi \sum_{l=1}^{n_c} \sigma_l \gamma_l}, \quad (4.14)$$

which, for $\gamma = 0$ and from equation (1.54), is equal to $|\alpha_{k|j}|^2$, and is centered at $k \approx \lambda_j t_0/(2\pi)$. Nevertheless, when $\gamma \neq 0$, the phase is shifted and the final distribution is not centered around the correct value. This problem is avoided by measuring the clock in the computational basis and postselecting the outcome $\gamma = 0$, as discussed in the next section.

4.2 Improved HHL variant

We have shown that the *HHL variant* becomes unreliable when the condition number is poorly estimated. An *improved HHL variant*, that is accurate even without any bound κ' , can be implemented with the amplitude amplification [99, 102] of the component $|1\rangle_a|0\rangle_c$, instead of $|1\rangle_a$, after the circuit that leads to the state (1.52). The probability $\tilde{p}$ of measuring $|1\rangle_a|0\rangle_c$ from the state (1.52) is

$$\tilde{p} = \sum_j |\beta_j|^2 \left(\sum_{k=k_{\min}}^{T-1} |\alpha_{k|j}^{\text{var}}|^2 \frac{CtT}{2\pi k} \right)^2. \quad (4.15)$$

The amplitude amplification will require an average number of calls to the circuit in Figure 1.1 of order $\sqrt{1/\tilde{p}}$. We are more restrictive on the state component to be amplified, $\tilde{p} < p_0$, but the bound (4.11) and $C = 2\pi k_{\min}/t_0 \simeq 1/(2\kappa')$ prove that $\tilde{p}$ and p_0 are both of order $\mathcal{O}(\lambda_{\min} \kappa')^{-2} = \mathcal{O}(\kappa/\kappa')^2$. Therefore, the *HHL variant* and the improved algorithm require the same number of calls to the circuit in Figure 1.1.

After the amplitude amplification of the state $|1\rangle_a|0\rangle_c$, the output state is

$$|\tilde{x}_0\rangle = \frac{1}{\sqrt{\tilde{p}}} \sum_j \sum_{k=k_{\min}}^{T-1} \beta_j |\alpha_{k|j}^{\text{var}}|^2 \frac{CtT}{2\pi k} |1\rangle_a|0\rangle_c |u_j\rangle_r. \quad (4.16)$$

In analogy to the state (4.1) that encodes the exact solution $\mathbf{x}$ (1.45) in the Hilbert space of quantum registers, the state (4.16) encodes the approximate solution $\tilde{\mathbf{x}} = \sum_j \beta_j \sum_{k=k_{\min}}^{T-1} |\alpha_{k|j}^{\text{var}}|^2 \frac{tT}{2\pi k} \mathbf{u}_j$.

The following theorem shows that the distance between the ideal output and the output of the *improved HHL variant* actually converges to zero for large T independently of κ' .

Theorem 4.2.1 (Lower bound on the convergence of the *HHL variant*). *Given the ideal output of the HHL algorithm (4.1) and the output state of the improved HHL variant (4.16), with coefficients $\alpha_{k|j}^{\text{var}}$ given by (1.54), the distance between these states is upper bounded by*

$$d(|x\rangle, |\tilde{x}_0\rangle) \leq \mathcal{O}\left(\frac{\kappa}{T} \ln \frac{T}{\kappa}\right). \quad (4.17)$$

Proof. We start by computing the fidelity between $|\tilde{x}_0\rangle$ and $|x\rangle$,

$$\begin{aligned} \langle x|\tilde{x}_0\rangle &= \frac{C^2}{\sqrt{p\bar{p}}} \sum_{j=0}^{2^n-1} \frac{|\beta_j|^2}{\lambda_j} \sum_{k=1}^{T-1} |\alpha_{k|j}^{\text{var}}|^2 \frac{tT}{2\pi k} \\ &= \frac{\sum_j \frac{|\beta_j|^2}{\lambda_j} \sum_{k=1}^{T-1} |\alpha_{k|j}^{\text{var}}|^2 \frac{tT}{2\pi k}}{\sqrt{\sum_j \frac{|\beta_j|^2}{\lambda_j^2} \sum_l |\beta_l|^2 \left(\sum_{k=1}^{T-1} |\alpha_{k|l}^{\text{var}}|^2 \frac{tT}{2\pi k}\right)^2}}. \end{aligned} \quad (4.18)$$

Using the definition (4.8) we obtain

$$d(|x\rangle, |\tilde{x}_0\rangle) = \sqrt{\frac{\sum_{j,l=0}^{2^n-1} \frac{|\beta_j|^2 |\beta_l|^2}{\lambda_j^2 \lambda_l^2} ((\epsilon_{1,j}^{\text{var}})^2 + \epsilon_{1,j}^{\text{var}} - \epsilon_{1,l}^{\text{var}} - \epsilon_{1,j}^{\text{var}} \epsilon_{1,l}^{\text{var}})}{\sum_{j,l=0}^{2^n-1} \frac{|\beta_j|^2 |\beta_l|^2}{\lambda_j^2 \lambda_l^2} (1 + \epsilon_{1,j}^{\text{var}})^2}}. \quad (4.19)$$

Observe that $d(|x\rangle, |\tilde{x}_0\rangle)$ depends only on $\epsilon_{1,j}^{\text{var}}$ and not on $\epsilon_{2,j}^{\text{var}}$, then its convergence is independent of κ' . Furthermore, the linear terms $\epsilon_{1,j}^{\text{var}} - \epsilon_{1,l}^{\text{var}}$ vanish by symmetry under exchange of dummy indices. Replacing $\epsilon_{1,j}^{\text{var}}$ with the asymptotic upper bound provided by Lemma 4.1.2, we find that the worst-case error is maximized by the smallest eigenvalue in the spectrum. Since the matrix A is scaled such that its maximum eigenvalue is a constant $\lambda_{\max} = \mathcal{O}(1)$, the minimum eigenvalue is order $\lambda_{\min} = \mathcal{O}(\kappa^{-1})$. Substituting this into the bound yields a maximum error scaling of $\mathcal{O}\left(\frac{\kappa}{T} \ln \frac{T}{\kappa}\right)$, and this concludes the proof. $\square$

Theorem 4.2.1 shows that the error can be arbitrarily small by choosing a big enough number of qubits n_c in the c register, with $T = 2^{n_c}$, provided that the condition number κ is not as large as T .

The quantum states $|\tilde{x}_0\rangle$ and $|x\rangle$ have unit normalization. In this sense, the states $|x\rangle$ and $|\tilde{x}_0\rangle$ encode only the direction of the vectors $\mathbf{x}$ and $\tilde{\mathbf{x}}$ respectively. Nevertheless, the norms of the vectors $\tilde{\mathbf{x}}$ and $\mathbf{x}$ defined above are

$$\|\tilde{\mathbf{x}}\|_2 = \frac{\sqrt{\tilde{p}}}{C}, \quad \|\mathbf{x}\|_2 = \frac{\sqrt{p}}{C}. \quad (4.20)$$

The probability $\tilde{p}$ can be measured implementing the amplitude estimation algorithm (a combination of the amplitude amplification and the quantum phase estimation algorithms) [99, 102] that uses an average number of calls to the circuit of Figure 1.1 of order $1/\sqrt{\tilde{p}}$. In order to prove that $\|\tilde{\mathbf{x}}\|_2$ well approximates $\|\mathbf{x}\|_2$, use equation (4.11) and $\lambda_{\min} = \min_j \lambda_j$ to compute

$$\frac{|\|\mathbf{x}\|_2^2 - \|\tilde{\mathbf{x}}\|_2^2|}{\|\mathbf{x}\|_2^2} \leq \frac{\sum_j \frac{|\beta_j|^2}{\lambda_j^2} |\epsilon_{1,j}^{\text{var}}|}{\sum_j \frac{|\beta_j|^2}{\lambda_j^2}} = \mathcal{O}\left(\frac{\ln(\lambda_{\min} t T)}{\lambda_{\min} t T}\right). \quad (4.21)$$

The bound (4.21) proves that the norm of the solution can be measured with arbitrary small error and with the same running time scaling required for the amplification of the amplitude of state $|\tilde{x}_0\rangle$.

The components of $\mathbf{x}$ cannot be computed efficiently using this algorithm, as discussed in subsection 1.4.1. Nevertheless, the algorithm allows to efficiently compute expectation values $\mathbf{x}^T M \mathbf{x}$ if M is a matrix that can be efficiently implemented on a quantum computer. In order to prove it, assume without loss of generality that M is Hermitian with eigenvalues $\{m_j\}_{j=1,\dots,d}$ and eigenvectors $\{\mathbf{m}_j\}_{j=1,\dots,d}$, otherwise apply the following argument to the Hermitian and the anti-Hermitian part of M independently.

Perform then a projective measurement on the output of the algorithm, $|\tilde{x}_0\rangle$, with projectors $\{|m_j\rangle\langle m_j|\}_{j=0,\dots,T-1}$. After μ of such measurements, the statistical frequency of obtaining the outcome m_j approximates the probability $|\langle \tilde{x}_0 | m_j \rangle|^2$ up to an error δ with probability $1 - \mathcal{O}(e^{-2\mu\delta^2})$ from the Chernoff-Hoeffding bound [169, 170]. When the sampling error δ is comparable with the computational errors (4.17), one requires $\mu > \mathcal{O}(\lambda_{\min} t T / \ln(\lambda_{\min} t T))$ repetitions for a good success probability in the Chernoff-Hoeffding bound. These repetitions can however be parallelized, without then increasing the computational time.

From the frequency of obtaining the state $|m_j\rangle$ and from the measurement of the norm discussed above, one computes

$$\|\tilde{\mathbf{x}}\|_2^2 \sum_{j=0}^{T-1} m_j |\langle \tilde{x}_0 | m_j \rangle|^2 = \|\tilde{\mathbf{x}}\|_2^2 \langle \tilde{x}_0 | M | \tilde{x}_0 \rangle = \tilde{\mathbf{x}}^T M \tilde{\mathbf{x}} = \mathbf{x}^T M \mathbf{x} \left(1 + \mathcal{O}\left(\frac{\ln(\lambda_{\min} t T)}{\lambda_{\min} t T}\right)\right), \quad (4.22)$$

achieving a good estimate of $\mathbf{x}^T M \mathbf{x}$ for large T .

4.3 Complexity

We analyze and compare here the complexity of the above algorithms. The relevant parameters for this analysis are the dimension d of the linear problem, the tolerance on the computational error ϵ , the condition number $\kappa = \max_j |\lambda_j| / \min_j |\lambda_j|$ of the matrix A , and its sparsity s which is the maximum number of non-vanishing elements in each row.

The number of qubits in the clock register n_c fix the value $T = 2^{n_c}$, and it is chosen such that the computational error, measured by the distance to the ideal state (4.3), is smaller than ϵ . The upper bound on the condition number κ' is chosen in the following way: if an estimate of the condition number is computed one can choose $\kappa' = \mathcal{O}(\kappa)$ independent of T . But, in the worst case, when no information of κ is available, and $k_{\min} = 1$, it scales as $\kappa' = \mathcal{O}(T)$.

Following Figure 1.1, the algorithm requires the following number of single-qubit gates, two-qubits gates and queries to the elements of the matrix A : As discussed in subsection 1.4.1, the operator $\mathcal{C}^{\text{var}}$ or $\mathcal{C}^{\text{HHL}}$ require $\mathcal{O}(\log_2 T)$ gates, with the difference that the first one can be completely parallelized and execute with circuit depth one. The simulation of the controlled gates (1.50) within error ϵ' in the quantum phase estimation can be done following the simulation algorithm [84, 85] described in section 1.4 with a number $\mathcal{O}(sT + \frac{\ln(1/\epsilon')}{\ln \ln(1/\epsilon')})$ of queries to the matrix elements of A and additional $\mathcal{O}(sT \ln d + \frac{\ln(1/\epsilon')}{\ln \ln(1/\epsilon')} \ln d)$ one- and two-qubit gates. We have used the assumption $0 < \lambda_j \leq 1$, which implies ¹ $\max_{i,j} |A_{i,j}| \leq 1$. The implementation of the quantum Fourier transform requires a number $\mathcal{O}(\log_2^2 T)$ of one- and two- qubit gates [75, 171] and the controlled rotations (1.51) require $\mathcal{O}(T \log_2^2 T)$ of such operations (see section A.1). We assume that the encoding of $\mathbf{b}$ can be done efficiently, and its time complexity is not considered here. Moreover, in order to implement the postselection, the circuit in Figure 1.1 has to be executed in average a number of times $\mathcal{O}(1/\sqrt{p_0})$ for the *original HHL algorithm* and the *HHL variant* or a number of times $\mathcal{O}(1/\sqrt{\tilde{p}})$ for the *improved HHL variant*. In any case, it is repeated $\mathcal{O}(\kappa'/\kappa)$ times to implement the postselection.

Putting all of this together, the number of sequential queries, also called *query complexity* is $\mathcal{Q} = \mathcal{O}(sT \kappa'/\kappa)$, and the number of consecutive additional gates, also called *gate complexity*, is $\mathcal{G} = \mathcal{O}((s \log_2 d + \log_2^2 T) T \kappa'/\kappa)$. We focus on the gate complexity as the query complexity is proportional to $\mathcal{G}$ up to logarithmic corrections. We will use the notation $\tilde{\mathcal{O}}(\cdot)$ to denote orders $\mathcal{O}(\cdot)$ up to multiplicative powers of the logarithm of its argument.

Consider the *improved HHL variant*. From Theorem 4.2.1, the error scales as $\tilde{\mathcal{O}}(\kappa/T)$. Replacing $T = \tilde{\mathcal{O}}(\kappa/\epsilon)$ into the gate complexity we obtain

¹The spectral decomposition of A is $A = \sum_l \lambda_l |u_l\rangle\langle u_l|$, and, using the Cauchy-Schwarz inequality, $|A_{ij}| = |\sum_l \langle e_i | u_l \rangle \lambda_l \langle u_l | e_j \rangle| \leq \sqrt{\sum_l |\langle e_i | u_l \rangle|^2 \lambda_l} \sqrt{\sum_l |\langle e_j | u_l \rangle|^2 \lambda_l} \leq \max_l \{\lambda_l\}$.

$$\tilde{\mathcal{G}}^{\text{var}} = \tilde{\mathcal{O}}\left(\frac{\kappa' s \log_2 d}{\epsilon}\right). \quad (4.23)$$

Consider the *HHL variant* applied with a proper estimation of the condition number ($\kappa' = \mathcal{O}(\sqrt{T\kappa \ln T/\kappa})$) to guaranty its convergence. From Theorem 4.1.1, the error scales as $\tilde{\mathcal{O}}(\sqrt{\kappa/T})$. Replacing $T = \tilde{\mathcal{O}}(\kappa/\epsilon^2)$ into the gate complexity we obtain

$$\mathcal{G}^{\text{var}} = \tilde{\mathcal{O}}\left(\frac{\kappa' s \log_2 d}{\epsilon^2}\right). \quad (4.24)$$

For the original *HHL algorithm*, from (4.4), we can replace $T = \mathcal{O}(\kappa/\epsilon)$, and obtain the gate complexity

$$\mathcal{G}^{\text{HHL}} = \tilde{\mathcal{O}}\left(\frac{\kappa' s \log_2 d}{\epsilon}\right). \quad (4.25)$$

Observe that (4.25) improves over the running time reported in [33]. It scales linearly in s , instead of quadratically, because we consider a more recent hamiltonian simulation algorithm, that gives this advantage. Also, it scales linearly in κ' , instead of quadratically, because we consider $T = \mathcal{O}(\kappa/\epsilon)$ instead of $T = \mathcal{O}(\kappa'/\epsilon)$.

In conclusion, the *improved HHL variant* has the same gate complexity as the *original HHL algorithm* up to logarithm corrections. Given a fixed number of qubits n_c in the clock, it requires lower depth in the clock initialization operator $\mathcal{C}$ at the price of a larger error in the output. The improved algorithm is more efficient than the HHL variant in terms of computational error, query and gate complexities. Furthermore, the improved algorithm is independent of having an estimate of the condition number, if we assume $k_{\min} = 1$ such that $1/\kappa' = 4\pi/t_0 = 4\pi/(tT)$ (see the discussion after equation (1.54)) scales as the machine precision, and thus eliminates the preprocessing time $\mathcal{O}(sd)$ required to obtain this estimate.

4.4 Numerical examples

In this section, we simulate the *HHL variant* and the improved algorithm for the solution of two dimensional linear problems ($d = 2$) using the python library qiskit, without implementing environmental noise on the quantum gates. The choice $d = 2$ allows us to consider larger numbers of qubits in the clock register $n_c \in [3, 11]$ without changing the error scaling with n_c . We then need only one qubit in the r -register, and fix the parameters, $k_{\min} = 1$, $t = 8\pi/5$ and $C = 2\pi/t_0$. The condition $k_{\min} = 1$ corresponds to the worst case scenario without any bound of the condition number.

For these numbers n_c , our classical simulation stores efficiently the full state vector, and then the amplitude amplifications is replaced by the readout of the corresponding state coefficient. The code can be found on GitHub².

²<https://github.com/MatiasGinzburg/Improvement-on-the-Convergence-in-Quantum-Linear-System->

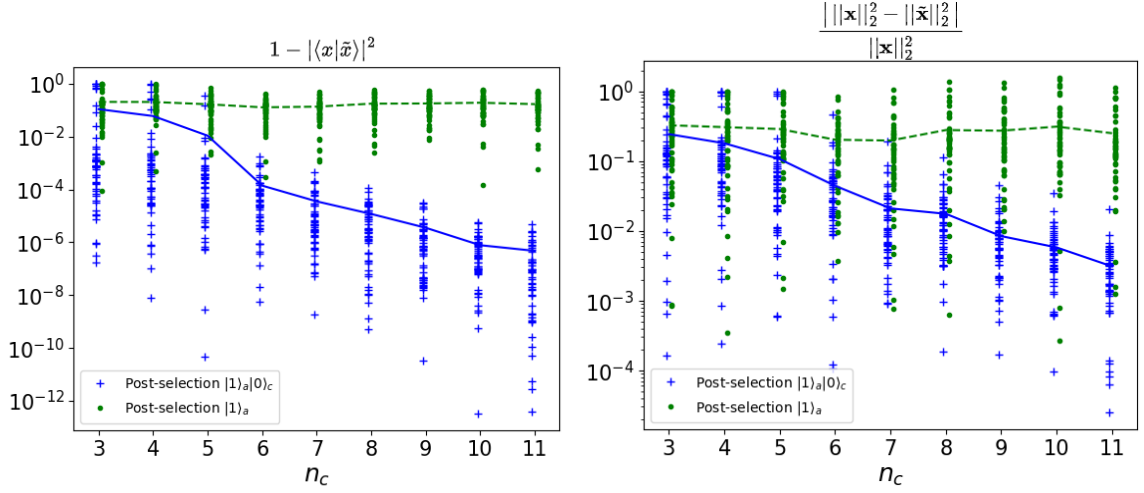


Figure 4.1: Log-lin plot of the infidelity (left panel) and of the norm error (right panel) between the output state and the ideal state of 50 randomly generated linear problems. Green dots corresponds to the *HHL variant* with postselection of the state $|1\rangle_a$, whose average behaviours are the dashed green lines. Blue crosses are the errors of the improved algorithm, and the solid blue lines are the averages.

We randomly generated 50 linear problems of the form (1.43) defined by Hermitian matrices A with eigenvalues in the range $(0, 1]$ and vectors b with unit norm. To generate such random matrices A , we sampled diagonal matrices $A' = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$ from the uniform distribution of $\lambda_j \in (0, 1]$ and transform them through a random unitary matrix, $A = UA'U^\dagger$, with U drawn from the Haar measure [172]. In Figure 4.1, we plot the infidelity (left panel) and the norm error (right panel) as function of the number n_c of qubits of the clock. We compared the *HHL variant* with postselection of the state $|1\rangle_a$ (green dots) and our improved algorithm with postselection of the state $|1\rangle_a|0\rangle_c$ (blue crosses), and the lines represent the average behaviors. The plots show that the errors of the *HHL variant* remain constant, while the errors of the new algorithm decrease to zero with increasing n_c , in agreement with the analytical computations in section 4.2.

4.5 Negative eigenvalues of A

In this section, we discuss how to apply the proposed algorithm to the case of non-positive eigenvalues of A . Using the normalization argument described in subsection 1.4.1, a general linear problem (1.43) is transformed into a linear problem with $-1 \leq \lambda_j \leq 1$.

First, set $t_0 = tT$ as before but with $0 < t < \pi$. After the phase estimation algorithm the distribution $|\alpha_{k|j}|^2$ is centered around $k \sim \lambda_j tT/(2\pi) \bmod T$. When the eigenvalue is positive $\lambda_j > 0$, the most probable value is $k \sim \lambda_j tT/(2\pi) < T/2$. When the eigenvalue is negative $\lambda_j < 0$, the most probable value is $k \sim \lambda_j tT/(2\pi) \bmod T > T/2$. In other words, the periodicity of the $\alpha_{k|j}$ is exploited to differentiate between positive and negative eigenvalues. Next, the angles $\theta(k)$ of the conditional rotation (1.51) are defined by

$$\sin(\theta(k)) := \begin{cases} \frac{C t_0}{2\pi k} & \text{if } k \leq T/2 \\ \frac{C t_0}{2\pi(k - T)} & \text{if } k \geq T/2 \end{cases}. \quad (4.26)$$

The bounds (4.11) and (4.12) hold true also for this case and so do all the conclusions. The difference in the computations arises in equation (A.7), where we should use the new equation (4.26). We also have to consider the cases $0 < t\lambda_j/(2\pi) < 1/2$ and $-1/2 < t\lambda_j/(2\pi) < 0$ separately in section A.2. There are divergences for $|t\lambda/(2\pi)| \approx 1/2$ which are avoided by choosing $t \neq \pi$. With this little modification, more general matrices can be handled.

4.6 Conclusions

We analyzed the *HHL algorithm* for solving linear systems (1.43) on quantum computers, as well as a variant algorithm that is often considered for practical implementations [104–108]. We focused on the scaling of the performances of these algorithms with the number of qubits n_c of the clock, which is a relevant parameter as it gives the precision of the quantum phase estimation for eigenvalue computations and the number of required gates. Another relevant parameter is the condition number that is usually assumed to have a known upper bound, and we extended the error analysis to the case where such bound is unknown. We proved that, in this case, the error of the *HHL variant*, unlike that of the original *HHL algorithm*, does not converge for large n_c but instead oscillates around a constant value. This non-convergent behavior arises from oscillatory terms in the amplified amplitude.

We proposed a modified algorithm based on the amplification of a smaller amplitude without detrimental oscillating terms. This modification preserves the simplicity of the original variant while restoring full convergence of the output error as the clock-register size increases. We confirmed this result with numerical simulations. Furthermore, the modified algorithm does not assume a bound of the condition number whose computation requires running time $\mathcal{O}(sd)$ and dominates the running time scaling with d of the quantum algorithm.

These findings are relevant for both theoretical developments and near-term implementations of quantum linear solvers as subroutines in larger quantum algorithms, particularly on NISQ platforms. In particular, practical implementations with currently available hard-

ware may not have sufficient gate depth and memory to implement more recent algorithms as those discussed in [86].

Appendix A

Detailed computations

We collect some detailed computations that are too long to include during the main presentation of chapter 4.

A.1 Steps of the HHL variant

In this appendix, we explicitly show intermediate states of the circuit in Figure 1.1. The first operator $\mathcal{C}$ is the initialization of the clock register that differentiates the original *HHL algorithm* from its variant, as discussed in section (1.4.1). The second gate (1.50) can be realized using the circuit represented in Figure A.1 [97] where each of the exponentials can be implemented if the matrix A is sparse or if it is a linear combination of unitaries [34, 36, 77–85]. The state after these operations is

$$|\psi_1^{\text{HHL}}\rangle = |0\rangle_a \sqrt{\frac{2}{T}} \sum_{j=0}^{2^n-1} \sum_{\tau=0}^{T-1} \beta_j \sin\left(\frac{\pi(2\tau+1)}{2T}\right) e^{i\frac{\tau}{T}\lambda_j t_0} |\tau\rangle_c |u_j\rangle_r, \quad (\text{A.1})$$

$$|\psi_1^{\text{var}}\rangle = |0\rangle_a \frac{1}{\sqrt{T}} \sum_{j=0}^{2^n-1} \sum_{\tau=0}^{T-1} \beta_j e^{i\frac{\tau}{T}\lambda_j t_0} |\tau\rangle_c |u_j\rangle_r, \quad (\text{A.2})$$

for the original *HHL algorithm* and for the *HHL variant* respectively.

After the inverse quantum Fourier transform the state vector can be written in the following compact form for both the *HHL algorithm* and the *HHL variant*,

$$|\psi_2\rangle = |0\rangle_a \sum_{j=0}^{2^n-1} \sum_{k=0}^{T-1} \beta_j \alpha_{k|j} |k\rangle_c |u_j\rangle_r, \quad (\text{A.3})$$

where the coefficients $\alpha_{k|j}$ are defined in equations (1.53) and (1.54). Since the state $|\psi_2\rangle$

has been achieved through unitary operations, it is normalized such that

$$1 = \langle \psi_2 | \psi_2 \rangle = \sum_{k=0}^{T-1} |\alpha_{k|j}|^2. \quad (\text{A.4})$$

The next gate, namely the controlled unitary defined by the transformation (1.51), can be implemented using $2^{n_c} - k_{\min}$ multi-qubit controlled rotations, as exemplified in Figure A.2. Each multi-qubit controlled rotation requires $\mathcal{O}(n_c^2)$ elementary gates [173], and thus the transformation (1.51) is implemented in time $\mathcal{O}(n_c^2 2^{n_c})$. The state vector after this step is

$$\begin{aligned} |\psi_3\rangle = & \sum_{j=0}^{2^n-1} \sum_{k=k_{\min}}^{T-1} \beta_j \alpha_{k|j} \sin(\theta(k)) |1\rangle_a |k\rangle_c |u_j\rangle_r \\ & + \sum_{j=0}^{2^n-1} \sum_{k=k_{\min}}^{T-1} \beta_j \alpha_{k|j} \cos(\theta(k)) |0\rangle_a |k\rangle_c |u_j\rangle_r \\ & + \sum_{j=0}^{2^n-1} \sum_{k=0}^{k_{\min}-1} \beta_j \alpha_{k|j} |0\rangle_a |0\rangle_c |u_j\rangle_r, \end{aligned} \quad (\text{A.5})$$

recalling $\sin \theta(k) := Ct_0/(2\pi k)$.

The quantum Fourier transform then yields the state vector

$$\begin{aligned} |\psi_4\rangle = & \frac{1}{\sqrt{T}} \sum_{j=0}^{2^n-1} \sum_{\sigma=0}^{T-1} \sum_{k=k_{\min}}^{T-1} \beta_j \alpha_{k|j} \sin(\theta(k)) e^{i\frac{\sigma}{T}2\pi k} |1\rangle_a |\sigma\rangle_c |u_j\rangle_r \\ & + \frac{1}{\sqrt{T}} \sum_{j=0}^{2^n-1} \sum_{\sigma=0}^{T-1} \sum_{k=k_{\min}}^{T-1} \beta_j \alpha_{k|j} \cos(\theta(k)) e^{i\frac{\sigma}{T}2\pi k} |0\rangle_a |\sigma\rangle_c |u_j\rangle_r \\ & + \frac{1}{\sqrt{T}} \sum_{j=0}^{2^n-1} \sum_{\sigma=0}^{T-1} \sum_{k=0}^{k_{\min}-1} \beta_j \alpha_{k|j} |0\rangle_a |\sigma\rangle_c |u_j\rangle_r. \end{aligned} \quad (\text{A.6})$$

After the inverse of the transformation (1.50) and the last gate $\mathcal{C}^{-1}$, one obtains the state (1.52).

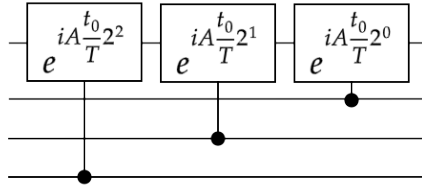


Figure A.1: Implementation of the conditional evolution operation for a clock with 3 qubits.

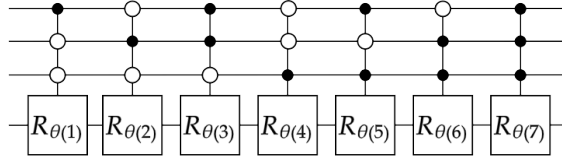


Figure A.2: Implementation of the conditional rotation described in equation (1.51) with $k_{\min} = 1$ and $n_c = 3$ qubits of the clock.

A.2 Proof of Lemma 4.1.2

In this appendix, we derive the bound (4.11). First, use the identity (A.4) and the triangle inequality to compute

$$\begin{aligned}
 |\epsilon_{1,j}| &= \lambda_j \left| \frac{1}{\lambda_j} - \sum_{k=k_{\min}}^{T-1} |\alpha_{k|j}^{\text{var}}|^2 \frac{tT}{2\pi k} \right| \\
 &= \left| \sum_{k=0}^{k_{\min}-1} |\alpha_{k|j}^{\text{var}}|^2 + \frac{\sin^2\left(\frac{\lambda_j tT}{2}\right)}{T^2} \sum_{k=k_{\min}}^{T-1} \frac{\left(k - \frac{\lambda_j tT}{2\pi}\right)}{k \sin^2\left(\frac{\pi}{T} \left(k - \frac{\lambda_j tT}{2\pi}\right)\right)} \right| \\
 &\leq \sum_{k=0}^{k_{\min}-1} |\alpha_{k|j}^{\text{var}}|^2 + \frac{\sin^2\left(\frac{\lambda_j tT}{2}\right)}{T^2} \sum_{k=k_{\min}}^{T-1} \frac{\left|k - \frac{\lambda_j tT}{2\pi}\right|}{k \sin^2\left(\frac{\pi}{T} \left(k - \frac{\lambda_j tT}{2\pi}\right)\right)}. \tag{A.7}
 \end{aligned}$$

In order to bound the sums in the right-hand-side of (A.7), we will extensively use the following inequalities

$$\sin(\pi x) \geq \begin{cases} 2x & \text{if } 0 \leq x \leq \frac{1}{2} \\ 2(1-x) & \text{if } \frac{1}{2} \leq x \leq 1 \end{cases}, \tag{A.8}$$

$$\sum_{x=a}^b f(x) \leq \int_a^b f(x) dx + f(a) + f(b), \tag{A.9}$$

valid for positive convex functions $f(x)$. The two cases in inequality (A.8) require to separately treat different contributions in the upper bound (A.7).

Let us start with considering $t\lambda_j/(2\pi) \leq 1/2$. The first term in (A.7) is bounded as

follows:

$$\begin{aligned}
\sum_{k=0}^{k_{\min}-1} |\alpha_{k|j}^{\text{var}}|^2 &= \sum_{k=0}^{k_{\min}-1} \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{T^2 \sin^2\left(\frac{\pi}{T}\left(\frac{\lambda_j t T}{2\pi} - k\right)\right)} \leq \frac{1}{4} \sin^2\left(\frac{\lambda_j t T}{2}\right) \sum_{k=0}^{k_{\min}-1} \left(\frac{\lambda_j t T}{2\pi} - k\right)^{-2} \\
&\leq \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{4} \left(\int_{k=0}^{k_{\min}-1} \left(\frac{\lambda_j t T}{2\pi} - k\right)^{-2} dk + \left(\frac{2\pi}{\lambda_j t T}\right)^2 + \left(\frac{\lambda_j t T}{2\pi} - k_{\min} + 1\right)^{-2} \right) \\
&\leq \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{4} \left(\frac{k_{\min} - 1}{\frac{\lambda_j t T}{2\pi} \left(\frac{\lambda_j t T}{2\pi} - k_{\min} + 1\right)} + \left(\frac{2\pi}{\lambda_j t T}\right)^2 + \left(\frac{\lambda_j t T}{2\pi} - k_{\min} + 1\right)^{-2} \right) \\
&\leq \frac{\pi}{2\lambda_j t T} + \left(\frac{2\pi}{\lambda_j t T}\right)^2 = \mathcal{O}\left(\frac{1}{\lambda_j t T}\right), \tag{A.10}
\end{aligned}$$

where we have used the assumption $1 \leq k_{\min} < \lambda_j t T / (4\pi)$ (see subsection 1.4.1) in the last inequality.

Defining $a_j = \lfloor \lambda_j t T / 2\pi \rfloor$ and $0 \leq \Delta_j < 1$ such that

$$\frac{\lambda_j t T}{2\pi} = a_j + \Delta_j, \tag{A.11}$$

the second sum in the upper bound (A.7) can be split into the following three sums

$$\sum_{k=k_{\min}}^{T-1} = \sum_{k=k_{\min}}^{a_j} + \sum_{k=a_j+1}^{a_j+\frac{T}{2}} + \sum_{k=a_j+\frac{T}{2}+1}^{T-1}. \tag{A.12}$$

Using again the inequalities (A.8) and (A.9), we compute for the first of these sums

$$\begin{aligned}
&\frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{T^2} \sum_{k=k_{\min}}^{a_j} \frac{\frac{\lambda_j t T}{2\pi} - k}{k \sin^2\left(\frac{\pi}{T}\left(\frac{\lambda_j t T}{2\pi} - k\right)\right)} \\
&\leq \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{4} \sum_{k=k_{\min}}^{a_j} \frac{1}{k \left(\frac{\lambda_j t T}{2\pi} - k\right)} \\
&\leq \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{4} \left(\int_{k_{\min}}^{a_j} \frac{1}{k \left(\frac{\lambda_j t T}{2\pi} - k\right)} dk + \frac{1}{k_{\min} \left(\frac{\lambda_j t T}{2\pi} - k_{\min}\right)} + \frac{1}{\Delta_j a_j} \right) \\
&= \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{4} \left(\frac{2\pi}{\lambda_j t T} \ln \left(\frac{a_j \left(\frac{\lambda_j t T}{2\pi} - k_{\min}\right)}{\Delta_j k_{\min}} \right) + \frac{1}{k_{\min} \left(\frac{\lambda_j t T}{2\pi} - k_{\min}\right)} + \frac{1}{\Delta_j a_j} \right) \\
&\leq \frac{\pi}{\lambda_j t T} \ln \left(\frac{\lambda_j t T}{2\pi} \right) + \frac{12\pi}{4\lambda_j t T} = \mathcal{O}\left(\frac{\ln(\lambda_j t T)}{\lambda_j t T}\right), \tag{A.13}
\end{aligned}$$

where we have used, in the last inequality, $\sin^2(\lambda_j t T / 2) = \sin^2(\pi \Delta_j)$, $0 < -\sin^2(\pi \Delta_j) \ln(\Delta_j) < 1$ and $\frac{\sin^2(\pi \Delta_j)}{\Delta_j} < 5/2$.

A very similar calculation bounds the second sum in (A.12):

$$\begin{aligned}
& \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{T^2} \sum_{k=a_j+1}^{\frac{T}{2}+a_j} \frac{k - \frac{\lambda_j t T}{2\pi}}{k \sin^2\left(\frac{\pi}{T}\left(k - \frac{\lambda_j t T}{2\pi}\right)\right)} \\
& \leq \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{4} \sum_{k=a_j+1}^{\frac{T}{2}+a_j} \frac{1}{k \left(k - \frac{\lambda_j t T}{2\pi}\right)} \\
& \leq \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{4} \left(\frac{4}{(T-2\Delta_j)(T+2a_j)} + \frac{1}{(1-\Delta_j)(a_j+1)} + \int_{a_j+1}^{\frac{T}{2}+a_j} \frac{1}{k \left(k - \frac{\lambda_j t T}{2\pi}\right)} dk \right) \\
& = \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{4} \left(\frac{4}{(T-2\Delta_j)(T+2a_j)} + \frac{1}{(1-\Delta_j)(a_j+1)} + \frac{2\pi}{\lambda_j t T} \ln \frac{(T-2\Delta_j)(a_j+1)}{(T+2a_j)(1-\Delta_j)} \right) \\
& \leq \frac{1}{4} \left(\frac{4}{T(T-2)} + \frac{10\pi}{2\lambda_j t T} - \frac{2\pi \ln 4}{\lambda_j t T} + \frac{2\pi}{\lambda_j t T} + \frac{2\pi}{\lambda_j t T} \ln \left(\frac{\lambda_j t T}{2\pi} + 1 \right) \right) \\
& = \mathcal{O} \left(\frac{\ln(\lambda_j t T)}{\lambda_j t T} \right). \tag{A.14}
\end{aligned}$$

The last inequality in equation (A.14) follows from the bounds $\frac{\sin^2(\pi \Delta_j)}{1-\Delta_j} < 5/2$, $-\sin^2(\pi \Delta_j) \ln(1-\Delta_j) < 1$, and $1/2 - 1/T < (T-2\Delta_j)/(T+2a_j) < 1$ which comes from $\lambda_j t/(2\pi) \leq 1/2$ and implies $|\ln(T-2\Delta_j)/(T+2a_j)| < \ln 4$ for $T \geq 4$.

Repeating the same procedure, the contribution from the last sum in (A.12) is

$$\begin{aligned}
& \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{T^2} \sum_{k=\frac{T}{2}+a_j+1}^{T-1} \frac{k - \frac{\lambda_j t T}{2\pi}}{k \sin^2\left(\frac{\pi}{T}\left(k - \frac{\lambda_j t T}{2\pi}\right)\right)} \\
& \leq \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{4} \sum_{k=\frac{T}{2}+a_j+1}^{T-1} \frac{k - \frac{\lambda_j t T}{2\pi}}{k \left(T + \frac{\lambda_j t T}{2\pi} - k\right)^2} \\
& \leq \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{4} \left(\frac{T-1 - \frac{\lambda_j t T}{2\pi}}{(T-1)\left(\frac{\lambda_j t T}{2\pi} + 1\right)^2} + \frac{4(T+2-2\Delta_j)}{(T+2\Delta_j-2)^2(T+2a_j+2)} \right. \\
& \quad \left. + \int_{\frac{T}{2}+a_j+1}^{T-1} \frac{k - \frac{\lambda_j t T}{2\pi}}{k \left(T + \frac{\lambda_j t T}{2\pi} - k\right)^2} dk \right) \\
& = \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{4} \left(\frac{T-1 - \frac{\lambda_j t T}{2\pi}}{(T-1)\left(\frac{\lambda_j t T}{2\pi} + 1\right)^2} + \frac{4(T+2-2\Delta_j)}{(T+2\Delta_j-2)^2(T+2a_j+2)} \right. \\
& \quad \left. + \frac{T}{T + \frac{\lambda_j t T}{2\pi}} \left(\frac{1}{\frac{\lambda_j t T}{2\pi} + 1} - \frac{2}{T+2\Delta_j-2} \right) + \frac{\frac{\lambda_j t T}{2\pi}}{\left(T + \frac{\lambda_j t T}{2\pi}\right)^2} \ln \frac{\left(\frac{\lambda_j t T}{2\pi} + 1\right)(T+2a_j+2)}{(T-1)(T+2\Delta_j-2)} \right) \\
& \leq \frac{1}{4} \left(\left(\frac{2\pi}{\lambda_j t T} \right)^2 + \frac{4}{T^2} + \frac{2\pi}{\lambda_j t T} + \frac{2\pi}{\lambda_j t T} \ln \left(2 \left(\frac{\lambda_j t T}{2\pi} + 1 \right) \frac{T+1}{(T-1)^2} \right) \right) \\
& = \mathcal{O}\left(\frac{1}{\lambda_j t T}\right). \tag{A.15}
\end{aligned}$$

Finally, the estimates (A.10), (A.13), (A.14), and (A.15) imply (4.11) for $0 < t\lambda_j/(2\pi) \leq 1/2$.

The second sum in the right-hand-side of (A.7) for the remaining case $1/2 < t\lambda_j/(2\pi) < 1$ is bounded following the same steps. Split the sum as

$$\sum_{k=k_{\min}}^{T-1} = \sum_{k=k_{\min}}^{a_j - \frac{T}{2}} + \sum_{k=a_j - \frac{T}{2} + 1}^{a_j} + \sum_{k=a_j+1}^{T-1}, \tag{A.16}$$

and use the inequalities (A.8) and (A.9) appropriately. The bound of the first sum in the

right-hand-side of (A.16) is

$$\begin{aligned}
& \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{T^2} \sum_{k=k_{\min}}^{a_j - \frac{T}{2}} \frac{\frac{\lambda_j t T}{2\pi} - k}{k \sin^2\left(\frac{\pi}{T} \left(\frac{\lambda_j t T}{2\pi} - k\right)\right)} \leq \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{4} \sum_{k=k_{\min}}^{a_j - \frac{T}{2}} \frac{\frac{\lambda_j t T}{2\pi} - k}{k \left(T + k - \frac{\lambda_j t T}{2\pi}\right)^2} \\
& \leq \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{4} \left(\frac{\frac{\lambda_j t T}{2\pi} - k_{\min}}{k_{\min} \left(T + k_{\min} - \frac{\lambda_j t T}{2\pi}\right)^2} + \frac{4(T + 2\Delta_j)}{(T - 2\Delta_j)^2 (2a_j - T)} \right. \\
& \quad \left. + \int_{k=k_{\min}}^{a_j - \frac{T}{2}} \frac{\frac{\lambda_j t T}{2\pi} - k}{k \left(T + k - \frac{\lambda_j t T}{2\pi}\right)^2} dk \right) \\
& = \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{4} \left(\frac{\frac{\lambda_j t T}{2\pi} - k_{\min}}{k_{\min} \left(T + k_{\min} - \frac{\lambda_j t T}{2\pi}\right)^2} + \frac{4(T + 2\Delta_j)}{(T - 2\Delta_j)^2 (2a_j - T)} \right. \\
& \quad \left. + \frac{T}{T - \frac{\lambda_j t T}{2\pi}} \left(\frac{2}{T - 2\Delta_j} - \frac{1}{T - \frac{\lambda_j t T}{2\pi} + k_{\min}} \right) \right. \\
& \quad \left. + \frac{\frac{\lambda_j t T}{2\pi}}{\left(T - \frac{\lambda_j t T}{2\pi}\right)^2} \ln \left(\frac{(2a_j - T) \left(T - \frac{\lambda_j t T}{2\pi} + k_{\min}\right)}{k_{\min} (T - 2\Delta_j)} \right) \right) \\
& = \mathcal{O}\left(\frac{\ln T}{T}\right). \tag{A.17}
\end{aligned}$$

This bound shows terms that diverge when $\lambda_j t / (2\pi)$ approaches 1, but the divergence is avoided by choosing $\max_j \lambda_j < 1$ and $t < 2\pi$. Indeed, t is a free parameter of the algorithm, and $\max_j \lambda_j < 1$ can be achieved by a rescaling of the linear problem as discussed in subsection 1.4.1.

The other two sums in the right-hand-side of (A.16) are bounded following very similar computations. Finally, we obtain equation (4.11) for any value $0 < \lambda_j t / (2\pi) < 1$.

A.3 Proof of Lemma 4.1.3

In this appendix, we compute the upper and lower bounds in equation (4.12). These bounds show the dependence of the computational error on the algorithm parameters T and $k_{\min}$. In particular, the error does not decrease with T when $k_{\min} = \mathcal{O}(T^0)$ which corresponds to a lower bound of the conditional number $\kappa' = tT / (2\pi k_{\min}) = \mathcal{O}(T)$.

We start with upper bounding the error contribution (4.9) using the triangle inequality,

$$\begin{aligned}
|\epsilon_{2,j}| &= \lambda_j^2 \left| \sum_{k=k_{\min}}^{T-1} |\alpha_{k|j}^{\text{var}}|^2 \left(\frac{tT}{2\pi k} \right)^2 - \frac{1}{\lambda_j^2} \right| \\
&\leq \sum_{k=0}^{k_{\min}-1} |\alpha_{k|j}^{\text{var}}|^2 + \frac{\sin^2 \left(\frac{\lambda_j tT}{2} \right)}{T^2} \sum_{k=k_{\min}}^{T-1} \frac{\left| \frac{\lambda_j tT}{2\pi} - k \right| \left(\frac{\lambda_j tT}{2\pi} + k \right)}{k^2 \sin^2 \left(\frac{\pi}{T} \left(\frac{\lambda_j tT}{2\pi} - k \right) \right)}. \tag{A.18}
\end{aligned}$$

The first sum is bounded by $\mathcal{O}(\lambda_j tT)^{-1}$, as shown in equation (A.10). In order to bound the second sum, we follow the same steps as in the previous appendix. For concreteness, we show only the case $\lambda_j t/(2\pi) < 1/2$, because the other case is very similar. Splitting the sum as in equation (A.12) and recalling the notation (A.11), the first contribution is the largest one and is bounded as follows

$$\begin{aligned}
&\frac{\sin^2 \left(\frac{\lambda_j tT}{2} \right)}{T^2} \sum_{k=k_{\min}}^{a_j} \frac{\left| \frac{\lambda_j tT}{2\pi} - k \right| \left(\frac{\lambda_j tT}{2\pi} + k \right)}{k^2 \sin^2 \left(\frac{\pi}{T} \left(\frac{\lambda_j tT}{2\pi} - k \right) \right)} \leq \frac{\sin^2 \left(\frac{\lambda_j tT}{2} \right)}{4} \sum_{k=k_{\min}}^{a_j} \frac{k + \frac{\lambda_j tT}{2\pi}}{k^2 \left(\frac{\lambda_j tT}{2\pi} - k \right)} \\
&\leq \frac{\sin^2 \left(\frac{\lambda_j tT}{2} \right)}{4} \left(\int_{k_{\min}}^{a_j} \frac{k + \frac{\lambda_j tT}{2\pi}}{k^2 \left(\frac{\lambda_j tT}{2\pi} - k \right)} dk + \frac{a_j + \frac{\lambda_j tT}{2\pi}}{\Delta_j a_j^2} + \frac{\frac{\lambda_j tT}{2\pi} + k_{\min}}{k_{\min}^2 \left(\frac{\lambda_j tT}{2\pi} - k_{\min} \right)} \right) \\
&= \frac{\sin^2 \left(\frac{\lambda_j tT}{2} \right)}{4} \left(\frac{4\pi}{\lambda_j tT} \ln \left(\frac{a_j \left(\frac{\lambda_j tT}{2\pi} - k_{\min} \right)}{k_{\min} \Delta_j} \right) \right. \\
&\quad \left. + \frac{a_j - k_{\min}}{k_{\min} a_j} + \frac{2a_j + \Delta_j}{\Delta_j a_j^2} + \frac{\frac{\lambda_j tT}{2\pi} + k_{\min}}{k_{\min}^2 \left(\frac{\lambda_j tT}{2\pi} - k_{\min} \right)} \right) \\
&\leq \mathcal{O} \left(\frac{\ln(\lambda_j tT)}{\lambda_j tT} \right) + \mathcal{O} \left(\frac{\kappa'}{tT} \right), \tag{A.19}
\end{aligned}$$

where we have used $(a_j - k_{\min})/(k_{\min}(a_j)) = \mathcal{O}(\kappa'/tT)$ in the last inequality. Using once again the same techniques, all the other terms coming from the splitting (A.12) are bounded by orders $\mathcal{O}(\ln(\lambda_j tT)/(\lambda_j tT))$. We then prove the upper bound in equation (4.12).

For the computation of the lower bound, we look again at the sum with $k \in [k_{\min}, a_j]$. Since all the terms are positive, we get a lower bound by neglecting all terms except

$k = k_{\min}$,

$$\begin{aligned}
& \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{T^2} \sum_{k=k_{\min}}^{a_j} \frac{\left(\frac{\lambda_j t T}{2\pi} - k\right) \left(\frac{\lambda_j t T}{2\pi} + k\right)}{k^2 \sin^2\left(\frac{\pi}{T} \left(\frac{\lambda_j t T}{2\pi} - k\right)\right)} \\
& \geq \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{k_{\min}^2 T^2} \cdot \frac{\left(\frac{\lambda_j t T}{2\pi} - k_{\min}\right) \left(\frac{\lambda_j t T}{2\pi} + k_{\min}\right)}{\sin^2\left(\frac{\pi}{T} \left(\frac{\lambda_j t T}{2\pi} - k_{\min}\right)\right)} \\
& \geq \frac{\sin^2\left(\frac{\lambda_j t T}{2}\right)}{\pi^2 k_{\min}^2} \cdot \frac{\frac{\lambda_j t T}{2\pi} + k_{\min}}{\frac{\lambda_j t T}{2\pi} - k_{\min}} \geq \sin^2\left(\frac{\lambda_j t T}{2}\right) \left(\frac{2\kappa'}{tT}\right)^2 \tag{A.20}
\end{aligned}$$

$$\geq \Omega\left(\frac{\kappa'}{T}\right). \tag{A.21}$$

All the other contributions of the splitting (A.12) are orders $\mathcal{O}(\ln(\lambda_j t T)/(\lambda_j t T))$. We then get the lower bound in equation (4.12).

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