



New architectures for solid-state quantum batteries: from theory to quantum simulation

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SUPERVISOR:
Prof. **Dario Ferraro**

CANDIDATE:
Giulia Gemme

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List of publications

This Thesis is based on the following papers co-authored by myself:

- **G. Gemme**, G. M. Andolina, Francesco M. D. Pellegrino, M. Sassetti, and D. Ferraro. *Off-Resonant Dicke Quantum Battery: Charging by Virtual Photons*. Batteries 9(4), 197 (2023).
- **G. Gemme**, M. Sassetti, and D. Ferraro. *Comparing different operating regimes of a Dicke quantum battery*. International Journal of Quantum Information 22(06), 2450024. (2024).
- **G. Gemme**, M. Grossi, S. Vallecorsa, M. Sassetti, and D. Ferraro. *Qutrit quantum battery: Comparing different charging protocols* Phys. Rev. Res. 6, 023091 (2024).
- L. Razzoli, **G. Gemme**, I. Khomchenko, M. Sassetti, H. Ouerdane, D. Ferraro, and G. Benenti. *Cyclic solid-state quantum battery: thermodynamic characterization and quantum hardware simulation*. Quantum Science and Technology 10, 015064 (2025).
- F. Cavaliere, **G. Gemme**, G. Benenti, D. Ferraro, and M. Sassetti. *Dynamical blockade of a reservoir for optimal performances of a quantum battery*. Communications Physics 8, 76 (2025)

Introduction

Batteries are fundamental components of nowadays technologies and play a crucial role in our daily lives. Varying greatly in size and capacity, they are devices capable of storing energy, supplied from an external system, and releasing it in a controlled manner to a user system. Despite the impressive technological improvements over the past two centuries, the batteries we currently use still rely on the electrochemical principles exploited by A. Volta at the end of the 18th century. However, the constant miniaturization of electronic devices calls for the realization of increasingly smaller batteries [1], down to sizes comparable to those of molecules and atoms. At these scales, quantum effects must be taken into account [2]. It is therefore necessary to reconsider energy manipulation within the framework of quantum thermodynamics [3–6], a research field that aims to extend the laws of classical thermodynamics and non-equilibrium statistical physics to systems where quantum effects become significant. In this context, the possibility to properly characterize the energetics of miniaturized thermal machines represented a major boost for the development of quantum technologies devoted to energy storage and manipulation.

One of the fundamental questions addressed by quantum thermodynamics is whether genuine quantum phenomena, such as entanglement and superposition of states, can give rise to energy storage devices with better performance than those achieved by classical batteries. The term *quantum battery* (QB) was introduced by R. Alicki and M. Fannes in 2013 to identify quantum devices in which energy can be temporarily stored for the purpose of transferring it from a producer system to a consumer one [7]. QBs are therefore quantum systems with non-degenerate energy levels, in which energy can be deposited (charging phase), stored and subsequently extracted (discharging phase). Both the charging and discharging processes occur by coupling the QB to an external system. In the charging phase, the external system supplies energy to the QB and is therefore referred to as the charger. In the discharging phase, energy is transferred from the QB to the user system or load. As will be seen later, not all the energy stored in the QB can always be extracted.

After the first appearance of the concept, these devices have seen an intense theoretical investigation, followed more recently by early experimental implementations. On the theoretical side, the first class of models considered as QB has been collections of two-level systems (TLSs) charged by means of quantum [7–22] or classical [23–26] external sources. Among those charged by a quantum source, it is worth mentioning the case of the Dicke QB, a collection of independent TLSs embedded in a resonant cavity, described by the Dicke model [10]. In these proposals the TLSs are devoted to the energy storage, while the photons in the cavity act as chargers. Among those charged by classical drives, we can mention QBs based on spin chains. In these systems, TLSs interact with one another. QBs based on these models can be charged via the action of a classical external field [27] or by quenching one or more

internal parameters [21] and can lead to long energy storage times [28–33]. However, in recent years, the possibility of addressing multilevel QBs to achieve high storage capacity has been discussed [34–36]. In this direction, one of the simplest and most versatile quantum systems is the quantum harmonic oscillator.

Building on these theoretical foundations, some experimental realizations have recently emerged. The first experiment was based on fluorescent molecules embedded within optical cavities, with an external laser playing the role of the charger [14]. The intensity of the matter-radiation interaction can be tuned here by changing the density of the molecules in the cavity. By increasing the number of trapped molecules (from 10^9 to 10^{12}), one observes a transition from a dissipation-dominated regime to the previously mentioned Dicke regime. With this system it is possible to achieve a quite stable energy storage, by properly exploiting the internal structure of the energy levels of the considered molecules, addressing fast decaying states for the charging and long-lived metastable state for the storage [37]. This kind of device has the great advantage of operating at room temperature, while their current major limitation is represented by the small overall storable energy with respect to classical counterparts. This is because it is not possible to pack too many molecules within the cavity without creating detrimental interactions among them. This could be overcome for example by using different elementary units such as inorganic molecules or nanoparticles [38]. Moreover, this architecture for QBs could strongly benefit for the impressive development of cavity engineered quantum materials [39, 40]. Another class of QB, based on nuclear spins in molecules, have been also developed. In these systems, the spin states are manipulated using time-dependent magnetic fields within the framework of nuclear magnetic resonance. As in previous case, these devices work at room temperature and are characterized by an extremely long time of energy storage [41, 42]. On a different front, cryogenic proof of principles of QBs also emerged. An important motivation behind these studies is the fact that QBs have been proposed as ingredient to realize a completely reversible and energy efficient quantum computation [43, 44]. In this direction solid-state implementations are emerging as natural candidates. These systems benefit from the ability to control both the charger and the coupling using conventional electronics, with response time in the nanosecond range, but are characterized by a very small amount of storable energy per qubit. In this context, energy storage devices based on superconducting circuits [24, 45] or quantum dots [46] and charged using a classical external source have been realized.

In this scenario, quantum simulations are gaining increasing relevance in the study of quantum technologies, as they occupy a unique position between theoretical models and experimental implementations. They offer a versatile framework to test hypotheses, explore system dynamics and validate predictions under controlled conditions, often anticipating or guiding future experimental efforts. In the context of QBs, simulations have enabled the analysis of charging dynamics and energy extraction processes. Experimental control of classical pulses in quantum computing platforms [47] has allowed investigations of qubits [25] and multi-level systems [26] as energy storage units. Simulations of thermodynamic cycles in a two-qubit QB [22] have highlighted a trade-off between maximizing extractable energy and minimizing operational costs. A recent work has also explored the role of continuous measurement and feedback in open QBs, showing how information gained from the environment can be used to enhance work extraction through optimized

quantum circuits [48]. All these simulation protocols have been implemented using IBM quantum computing platforms [49].

Within this framework, this Thesis will focus on various aspects of solid-state QBs. It is organized into five Chapters. The first two provide an overview of the theoretical framework required for the study of QB. Notably, the second Chapter begins to introduce also original results, which are presented as illustrative examples. The remaining three Chapters are devoted to the main original findings obtained during the course of the doctoral research. A brief overview of the contents of each chapter is provided below to guide the reader through the progression of the Thesis.

Chapter 1 introduces the fundamental elements, both theoretical and experimental, required for the study and implementation of TLSs. The first part presents the formalism used to describe the physics of TLSs and their time evolution [50]. The second part focuses on the concept of *qubit* [51, 52] and presents some of the most common platforms employed for the experimental realization of such devices [53]. The characteristics of qubits based on trapped ions [54, 55] and Rydberg atoms [56–58] are briefly described, while particular attention is given to superconducting qubits. This choice is motivated by the fact that they constitute the core technology of IBM quantum computers, which were used during the research activity.

Chapter 2 focuses on the theoretical modeling and performance analysis of QBs. It begins with the definition of a general framework for describing these systems, followed by a discussion about the main figures of merit used to evaluate their performances [59]. They include the stored energy, the average charging power, the ergotropy [60], namely the maximum amount of work that can be extracted via unitary operation, and the energetic cost of switching interactions on and off. In the second part of the Chapter, we examine specific models of QB, discussing also some original results: few-level QBs charged by classical fields, based on two- and three-level systems [25, 26], with a simulation on IBM quantum computers, and the Dicke QB, analyzing both resonant [10] and off-resonant [61, 62] regimes.

Chapter 3 reports the results published in Ref. [22]. We introduce a cyclic QB model, based on an interacting bipartite system, weakly coupled to a thermal bath. The working cycle of the battery consists of four strokes: system thermalization, disconnection of subsystems, ergotropy extraction, and reconnection. The thermal bath acts as a charger in the thermalization stroke, while ergotropy extraction is possible because the ensuing thermal state is no longer passive after the disconnection stroke. Focusing on the case of two interacting qubits, we show that phase coherence, in the presence of non-trivial correlations between the qubits, can be exploited to reach working regimes with efficiency higher than 50% while providing finite ergotropy. The protocol is illustrated through a simple and feasible circuit model of a cyclic superconducting QB. Furthermore, we have simulated the considered cycle on superconducting IBM quantum computers. The good agreement between the theoretical and simulated results strongly suggests that our scheme for cyclic quantum batteries can be successfully realized in superconducting quantum hardware.

Chapter 4 contains the results published in Ref. [36]. Here, the QB is modeled as a quantum harmonic oscillator, strongly coupled to a reservoir described as a large collection of quantum harmonic oscillators in the framework of the Caldeira-Leggett model [63, 64] and playing the role of the charger. The charging process relies on the transient dynamics, that occurs right after the battery is connected to

the quantum charger, enabling a fast charging protocol. We show that this protocol is very efficient, with the ergotropy closely matching the energy stored in the QB. These features are due to two key ingredients, the non-Markovianity of the reservoir, and a peculiar working regime where the reservoir is strongly coupled to the QB. Such QB model can be realized with a quantum LC circuit playing the role of the battery and with the required environment being suitably engineered via state-of-the-art quantum circuits.

Finally, **Chapter 5** describes a possible solid-state implementation of a Dicke QB, introduced in Chapter 2, based on a Josephson junction (JJ). In this framework, the QB consists of N TLSs, as in the standard Dicke model, with the key distinction that the TLSs correspond to the various transport channels of the junction, whose energy gaps are determined by their transmission coefficients. The model is initially developed for a generic JJ, without reference to specific material properties. Subsequently, the analysis focuses on the case of a graphene Josephson junction (GJJ), where the transmission probabilities are derived from the electronic spectrum of graphene. This leads to a dispersion relation governing the energy gaps of the TLSs composing the QB. The Chapter concludes with the investigation of the charging dynamics within this framework, emphasizing the influence of graphene-induced spectral features on the device's performance. The results of this study will be published in Ref. [65].

Few **Appendices (A to D)** are used to illustrate technical parts of the calculations and to discuss several details in support of the comments presented in the main text.

Chapter 1

Qubit

The aim of this Chapter is to introduce the basic theoretical and experimental elements necessary to study QBs. In the first part, the fundamental characteristics of TLSs, which constitute the basic physical building blocks of *qubits*, will be described, and subsequently, some of the state-of-the-art physical systems used to realize them will be introduced. Since part of this Thesis focuses on the study of simulations of QBs on IBM quantum computers, particular attention will be devoted to the discussion of qubits based on superconducting circuits, the technology employed by IBM.

1.1 Two-level systems

The elementary building block for a QB is the TLS [8]; therefore, it is first of all necessary to discuss the fundamental characteristics of these kind of quantum systems. The Hamiltonian $\hat{\mathcal{H}}$ that describes a TLS acts in a two-dimensional Hilbert space $\mathcal{h}$. A possible basis for defining the Hermitian operators acting in this space is the set of Pauli operators plus the identity, namely

$$\{\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z, \hat{\sigma}_0\}. \quad (1.1)$$

In the basis where $\hat{\sigma}_z$ is diagonal, its eigenstates are represented as

$$|0\rangle \rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |1\rangle \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (1.2)$$

The basis in Eq. (1.2), in the context of quantum technologies, is called the *computational basis*. In this basis, a generic state of the system can be written as

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle \quad (1.3)$$

with $|\alpha|^2 + |\beta|^2 = 1$.

In the computational basis, the operators in Eq. (1.1) are represented by the following matrices [50, 66]

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \hat{\sigma}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (1.4)$$

The main properties of the Pauli operators are

- $\text{Tr}\{\hat{\sigma}_i\} = 0$,
- $\det\{\hat{\sigma}_i\} = -1$,
- $[\hat{\sigma}_i, \hat{\sigma}_j] = 2i\epsilon_{ijk}\hat{\sigma}_k$,
- $\{\hat{\sigma}_i, \hat{\sigma}_j\} = 2\delta_{ij}$

with $i, j, k = x, y, z$. Finally, the following identity applies,

$$e^{i\phi\hat{\mathbf{n}}\cdot\hat{\boldsymbol{\sigma}}} = \hat{\sigma}_0 \cos \phi + i(\hat{\mathbf{n}} \cdot \hat{\boldsymbol{\sigma}}) \sin \phi \quad (1.5)$$

with $\hat{\mathbf{n}} \in \mathbb{R}^3$, $|\hat{\mathbf{n}}| = 1$, $\hat{\boldsymbol{\sigma}} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$, and $\phi \in \mathbb{R}$.

Since Eq. (1.1) is a basis of $\mathcal{h}$, the Hamiltonian of a TLS can be written as

$$\hat{\mathcal{H}} = \frac{1}{2} [\lambda_0 \hat{\sigma}_0 + \boldsymbol{\lambda} \cdot \hat{\boldsymbol{\sigma}}] \quad (1.6)$$

where $\boldsymbol{\lambda} = (\lambda_x, \lambda_y, \lambda_z)$. The constant term, $\lambda_0 \hat{\sigma}_0$, can be always reabsorbed by properly redefining the zero of energy.

Starting from Eq. (1.6), it is possible to compute the eigenstates and the energy spectrum of the system. The latter is given by the eigenvalues of the Hamiltonian in Eq. (1.6)

$$E_{\pm} = \frac{1}{2} [\lambda_0 \pm |\boldsymbol{\lambda}|] = \frac{1}{2} \left[\lambda_0 \pm \sqrt{\sum_{i=1}^3 \lambda_i^2} \right], \quad (1.7)$$

the corresponding eigenstates are

$$|\lambda_{\pm}\rangle = \mathcal{N}_{\pm} \left(\frac{\lambda_x - i\lambda_y}{\pm|\boldsymbol{\lambda}| - \lambda_z} |0\rangle + |1\rangle \right), \quad (1.8)$$

with $\mathcal{N}_{\pm}$ being a proper normalization constant.

Referring back to Eq. (1.3), it is often useful to express it in polar coordinates, where its form becomes [67]

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right) |0\rangle + e^{i\phi} \sin\left(\frac{\theta}{2}\right) |1\rangle \quad (1.9)$$

with $\theta \in [0, \pi]$ e $\phi \in [0, 2\pi]$. This leads to a natural geometric representation of the state of a TLS on a unit-radius sphere, the so called *Bloch sphere*, shown in Fig. 1.1.

The state described by Eq. (1.9) is represented by the unit vector $\mathbf{r} = (r_x, r_y, r_z)$ with $r_i = \langle\psi|\hat{\sigma}_i|\psi\rangle$. In the basis in Eq. (1.1) we have

$$r_x = \langle\psi|\hat{\sigma}_x|\psi\rangle = \left(\cos\frac{\theta}{2} \quad \sin\frac{\theta}{2}e^{-i\phi}\right) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \left(\cos\frac{\theta}{2} \quad \sin\frac{\theta}{2}e^{i\phi}\right)^T = \sin\theta \cos\phi \quad (1.10)$$

$$r_y = \langle\psi|\hat{\sigma}_y|\psi\rangle = \left(\cos\frac{\theta}{2} \quad \sin\frac{\theta}{2}e^{-i\phi}\right) \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \left(\cos\frac{\theta}{2} \quad \sin\frac{\theta}{2}e^{i\phi}\right)^T = \sin\theta \sin\phi \quad (1.11)$$

$$r_z = \langle\psi|\hat{\sigma}_z|\psi\rangle = \left(\cos\frac{\theta}{2} \quad \sin\frac{\theta}{2}e^{-i\phi}\right) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \left(\cos\frac{\theta}{2} \quad \sin\frac{\theta}{2}e^{i\phi}\right)^T = \cos\theta. \quad (1.12)$$

With this representation the north pole of the sphere represents the state $|0\rangle$ and the south pole the state $|1\rangle$. The states associated to the points on the Bloch sphere correspond to the pure states of a TLS [68]. These are the ones that can be described by a wave function. The points inside the sphere, instead, represent the mixed states of the system and must be described with a density operator. In the following Section, we will briefly outline its keys concepts [52, 66].

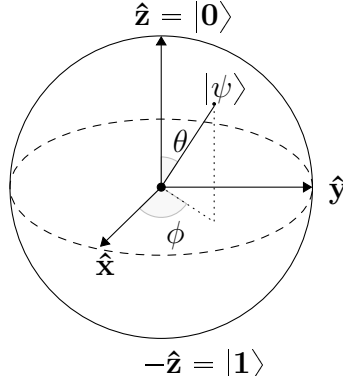


Figure 1.1: Bloch sphere representation of a qubit state $|\psi\rangle$ as described in Eq. (1.9).

1.1.1 Density Matrix

The wave function is a complete description of a closed quantum system, which is subjected to unitary dynamics. However, there are situations in which this level of detail is either not possible or not required. This situation arises, for example, in the description of a subsystem of a larger system: having access only to a part of the dynamical variables, it is not possible to describe the subsystem with a wave function. This is the typical case that occurs when describing a system interacting with an uncontrolled environment. Another important example concerns systems with many degrees of freedom like macroscopic systems, solids and gases. In these cases, it is obviously impossible to have complete knowledge of the wave function of (typically) 10^{23} molecules. All these cases are characterized by the partial lack of information about the system.

To describe such situation, we can consider a general closed system Σ and one of its subsystems, S . Let's call x the variables in S , to which we have access, and q the rest of the variables in Σ/S , that we do not know. The total system is described by a wave function $|\psi(q, x)\rangle$, but, in general, it is not possible to factorize it into a wave function defined on S and one on Σ/S ; that is

$$|\psi(q, x)\rangle \neq |\psi_S(x)\rangle \cdot |\psi_{\Sigma/S}(q)\rangle. \quad (1.13)$$

This means that the subsystem S does not have a wave function in general. Instead, the correct description of S is given by the definition of the density matrix, obtained by tracing out the unknown degrees of freedom q

$$\rho_S(x, x') = \int dq |\psi(q, x)\rangle \langle \psi(q, x')|. \quad (1.14)$$

This density matrix encodes all the accessible information about S . The density matrix is a Hermitian operator (considering x and x' as indices of a matrix)

$$\rho(x; x')^* = \rho(x'; x). \quad (1.15)$$

Moreover, it satisfies an important property

$$\text{Tr} \rho = \int dx \rho(x; x) = 1. \quad (1.16)$$

In applications, it is often necessary to evaluate the expectation value of an operator $\hat{f}$ that depends only on variables in the subsystem S . By definition, we have

$$f \equiv \langle \hat{f} \rangle = \langle \psi | \hat{f} | \psi \rangle = \int dq dx \langle \psi(q, x) | \hat{f}(x) | \psi(q, x') \rangle. \quad (1.17)$$

For the various applications we are interested in, it is more convenient to use a discrete basis $|n\rangle$ instead of the continuous one $|x\rangle$ used so far. Inserting completeness relations and integrating over the variables q , we obtain

$$f = \sum_{n,m} \int dq dq' \langle \psi | q, n \rangle \langle q, n | \hat{f} | q', m \rangle \langle q', m | \psi \rangle. \quad (1.18)$$

Since $\hat{f}$ acts only on the subsystem S , it does not affect the variable q , and we use

$$\langle q, n | \hat{f} | q', m \rangle = \langle n | \hat{f} | m \rangle \delta(q - q'). \quad (1.19)$$

This simplifies the expression to

$$f = \sum_{n,m} \int dq \langle \psi | q, n \rangle \langle n | \hat{f} | m \rangle \langle q, m | \psi \rangle. \quad (1.20)$$

We now define the reduced density matrix elements

$$\rho_{mn} \equiv \int dq \langle q, m | \psi \rangle \langle \psi | q, n \rangle \quad (1.21)$$

and the matrix elements of the operator

$$f_{nm} = \langle n | \hat{f} | m \rangle. \quad (1.22)$$

Thus, the expectation value becomes simply

$$f = \text{Tr}[\rho \hat{f}]. \quad (1.23)$$

In particular, this Equation can be applied to $\hat{f} = \hat{\sigma}_i$, with $i = x, y, z$. Doing this we can define

$$r_x = \text{Tr}[\hat{\sigma}_x \rho], \quad r_y = \text{Tr}[\hat{\sigma}_y \rho], \quad r_z = \text{Tr}[\hat{\sigma}_z \rho], \quad (1.24)$$

which are the coordinates of the state ρ on the Bloch sphere. The radius $r \equiv |\mathbf{r}| = \sqrt{r_x^2 + r_y^2 + r_z^2}$ is related to the purity of the state $\text{Tr}[\rho^2] = \frac{1}{2}(1 + r^2)$, ranging from $r = 0$ (maximally mixed state) to $r = 1$ (pure state), extending the notion introduced in the previous Section.

With this formalism, the more general state of a qubit is represented by the density matrix [69]

$$\rho = \frac{1}{2}(\hat{\sigma}_0 + \mathbf{r} \cdot \boldsymbol{\sigma}) = \frac{1}{2} \begin{pmatrix} 1 + r_z & r_x - ir_y \\ r_x + ir_y & 1 - r_z \end{pmatrix}. \quad (1.25)$$

Extending the results of the previous Section, the eigenvalues of ρ are $E_{\pm} = \frac{1}{2}(1 \pm r)$ and the corresponding eigenstates are

$$|\lambda_{\pm}\rangle = \mathcal{N}_{\pm} \left(\frac{r_x - ir_y}{\pm r - r_z} |0\rangle + |1\rangle \right). \quad (1.26)$$

Since $E_- \leq E_+$, as $0 \leq r \leq 1$, at thermal equilibrium the eigenstate $|\lambda_- \rangle$ is the least populated, and $|\lambda_+ \rangle$ the most populated.

1.1.2 Time Evolution

Another important idea that is crucial to study QBs is the time evolution of a quantum state. If the state is described by a wave function it is given by the Schrödinger equation [50]

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{\mathcal{H}}(t) |\psi(t)\rangle. \quad (1.27)$$

For a closed system, it is always possible to define an operator $\hat{\mathcal{U}}(t)$ such that

$$|\psi(t)\rangle = \hat{\mathcal{U}}(t) |\psi(0)\rangle. \quad (1.28)$$

In the case where $\hat{\mathcal{H}}$ does not explicitly depend on time, substituting this expression into Eq. (1.27) yields

$$\begin{aligned} i\hbar \frac{d}{dt} \hat{\mathcal{U}}(t) |\psi(0)\rangle &= \hat{\mathcal{H}} \hat{\mathcal{U}}(t) |\psi(0)\rangle \\ i\hbar \frac{d}{dt} \hat{\mathcal{U}}(t) &= \hat{\mathcal{H}} \hat{\mathcal{U}}(t) \\ \implies \hat{\mathcal{U}}(t) &= e^{-\frac{i}{\hbar} \hat{\mathcal{H}} t}. \end{aligned} \quad (1.29)$$

To treat time evolution, it is generally more convenient to work in the eigenbasis of the Hamiltonian; in this basis $\hat{\mathcal{H}}$ is diagonal, and consequently so is the operator $\hat{\mathcal{U}}(t)$, otherwise more involved strategies are needed [50]. In the case where the Hamiltonian explicitly depends on time, a similar reasoning to Eq. (1.29) can be applied only if $[\hat{\mathcal{H}}(t_1), \hat{\mathcal{H}}(t_2)] = 0$. When this commutator is non-zero, the definition of the time evolution operator requires the introduction of the time-ordering operator $\mathcal{T}$, leading to the expression

$$\hat{\mathcal{U}}(t, t_0) = \mathcal{T} \exp \left(-\frac{i}{\hbar} \int_{t_0}^t \hat{\mathcal{H}}(t') dt' \right) \quad (1.30)$$

Deriving Eq. (1.14) and substituting Eq. (1.27) in it, we can also get the equation that describe the evolution in time of the density matrix [50]

$$i\hbar \frac{d}{dt} \rho = -[\rho, \hat{\mathcal{H}}]. \quad (1.31)$$

1.2 Qubit: physical implementations

The TLS theoretically discussed above, also known as qubit (or quantum bit), is the fundamental building block of quantum technologies, serving as the quantum equivalent of the classical bit. Unlike a classical bit, which can only assume the values 0 or 1, a qubit exist in the bi-dimensional Hilbert space $\mathcal{h}$ introduced in the previous Section.

The aim of this Section is to describe the most common platforms currently used to build qubits [53]. They are generally grouped into two main categories: natural and artificial systems. In the former case, the TLS needed to have a qubit is identified in a physical system that already exists in nature. With this approach, qubits are intrinsically identical, they can be kept very well isolated from the environment, and

they are typically so small that only quantum physics can describe their behavior. On the other hand, it is not easy to modify their parameters and control them. In contrast, in the artificial system scenario, the goal is to build man-made devices that, under proper conditions, behave like qubits. This makes it possible to modify qubit parameters, even if within certain limits, even during operations and to harness quantum mechanical effects in “macroscopic” systems, that are usually easier to manipulate. The main drawbacks are that qubits can never be perfectly identical and are usually affected by noise and decoherence more than natural systems, because large and complex systems like them interact very strongly with the environment.

Having defined the two main categories of qubit technologies, we can now examine specific examples within each group, along with the companies currently leading their development. Among natural systems, trapped ions [54] represent the most developed technology so far, with the company ION Q [70] being the world leader in this field. In recent years, a promising alternative seems to be given by Rydberg atoms [56–58], with some companies that are working with them, such as Pasqal [71] and QuEra Computing [72]. Another example is given by photonic qubits [73], which can be based on several approach such as photon polarization, dual-rail scheme and time-bin encoding. A problem of this technology is that it is quite difficult to implement two-qubit operations since photons do not interact with each other. Among the companies that work with this technology we can mention Xanadu [74] and Quandela [75].

Concerning artificial systems, the most cutting-edge technology is represented by the superconducting qubits [53, 76–78], which utilize superconductive circuits and aim to operate via the cloud. Currently, the world leaders in this field are IBM [49], Google [79], and Rigetti [80]. In terms of scalability, semiconductor qubits are the most advanced platform. They are based on *quantum dots* [81, 82], potential wells that can only contain a finite number of electrons, and exploit the conventional semiconductor technology used to produce computer chips. This technology has not yet been commercialized due to challenges in manipulating coupled qubits. The leading company in this field is INTEL [83]. Finally, topological qubits [84], also known as Majorana zero modes, are still considered a futuristic platform aimed at realizing new states of matter with properties exploitable as qubits. Although they have not been realized yet, they promise immunity to various sources of decoherence and environmental noise. In this area, Microsoft is the leading actor [85].

In the following Sections of this Chapter, we will examine some of the previously mentioned systems used to implement qubits. Particular emphasis will be given to superconducting qubits, as this is the technology on which the quantum computers used during this Thesis to simulate QBs are based.

1.2.1 Trapped ions

In 1995, when the first quantum algorithms emerged, Ignacio Cirac and Peter Zoller proposed to build qubits using charged ions trapped in a small volume thanks to electromagnetic fields [54]. The use of charged ions instead of neutral atoms is justified by the relative simplicity of realize an electromagnetic confinement in this case [51, 55]. The idea is to use a set of N ions, interacting with laser light and confined in a linear trap. The TLS needed to have a qubit is identified within the energy spectrum of the ion, the choice usually includes the ground state, indicated

with $|0\rangle$, and an excited state, indicated with $|1\rangle$. Because of their atomic structure, the most commonly used elements for this kind of application are elements of the groups *IIA* and *IIB* such as *Be*, *Mg*, *Ca*, *Sr*, *Ba*, *Zn*, *Cd*, *Hg*, *Yb* [86]. The transition between $|0\rangle$ and $|1\rangle$ can be chosen either in the optical or in the hyperfine range [87, 88]. However, given that the lifetime of hyperfine qubits is much longer than the optical qubits and because hyperfine qubits are easier to manipulate, it is generally preferred to choose the latter. Currently, typical values for the lifetimes are $T_1, T_2 \sim 1$ s for optical qubits and $T_1, T_2 \sim 10$ min for hyperfine qubits. In this context, the relaxation time T_1 characterizes the decay of the population term σ_z toward its equilibrium value, while the dephasing time T_2 quantifies the decay of the coherences, associated with the σ_x and σ_y operators. The current state of the art of ion manipulation techniques allows rates of operation of 100 kHz allowing between 10^5 and 10^7 operations within this time span [87, 89]. All of this is true under conditions of high vacuum (at pressures of about 10^{-11} Torr $\sim 1.3 \cdot 10^{-9}$ Pa) [90, 91] and carefully shielding from possible uncontrolled radiation [86].

The most common traps are the so called Penning trap [92], where static electric and magnetic potentials are used and the Paul trap [93, 94], where static and oscillating electric fields are used. Although both are in principle suitable for quantum computing applications, the Paul trap is currently the most used method in both academy and industry. Two examples of Paul traps are shown in Fig. 1.2.

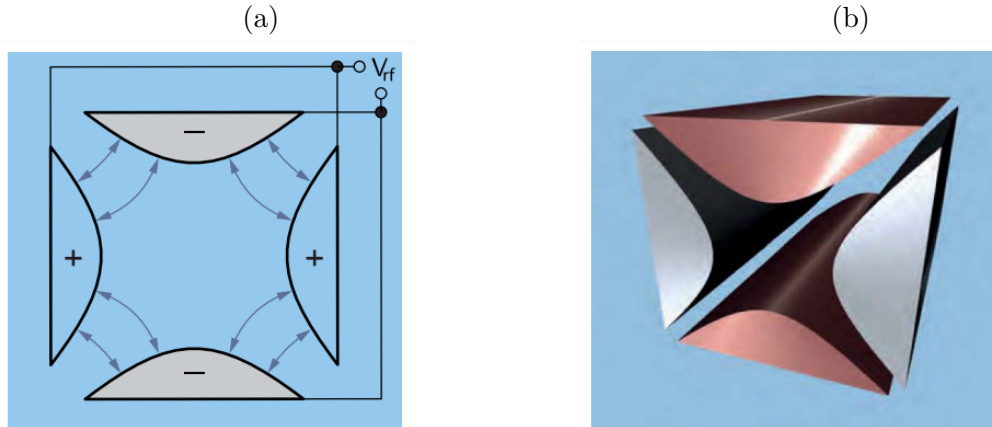


Figure 1.2: Examples of Paul trap geometries. (a) Simplest geometry capable of creating a quadrupolar field. (b) Linear trap, a translationally symmetric geometry that create a pseudopotential which confines in two directions. Image taken from [95] and adapted.

It is worth noting that the trap plays a dual role: it confines the ions within the desired volume and also serves as a mediator for implementing single- and two-qubit operations [95].

The net result is that the ions are located in a effective harmonic potential [51]

$$V(x, y, z) = \frac{1}{2}M(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \quad (1.32)$$

where M is the ion mass, $\mathbf{r} = (x, y, z)$ is its position and $\omega_x, \omega_y, \omega_z$ are the trap frequencies along the three orthogonal directions. The most commonly trapping systems used in quantum computing applications are linear traps, showed in panel (b),

where the frequencies satisfy the relation

$$\omega_x \simeq \omega_y \gg \omega_z \quad (1.33)$$

and where the typical order of magnitude of ω_z is ~ 1 MHz. It means that, at low energy, the motion of the ion remains frozen along x and y and the ion moves along the axis Oz , therefore the problem can be approximate with the following effective potential in one dimension

$$V(z) = \frac{1}{2}M\omega_z^2 z^2. \quad (1.34)$$

Considering only one ion, its coordinate $\hat{z}$ and the z component of the momentum $\hat{p}_z$, the Hamiltonian of the system can be written as

$$\hat{\mathcal{H}} = \hat{K} + \hat{V} = \frac{1}{2M}\hat{p}_z^2 + \frac{1}{2}M\omega_z^2 \hat{z}^2 \quad (1.35)$$

with $\hat{K}$ the kinetic energy. The previous approximation is consistent if the ion does not move appreciably away from the trap center, so it is necessary that the ion moves slowly, namely with a low kinetic energy. More quantitative, this inequality need to satisfy

$$k_B T \ll \hbar\omega_z, \quad (1.36)$$

with k_B the Boltzman constant, which implies that the temperature must satisfy $T \ll 10^{-5}$ K. It is therefore essential to maintain the system at extremely low temperatures. To achieve this, the method of *laser cooling* is used [86, 96].

Doppler cooling

The Doppler cooling is based, as the name suggests, on the Doppler effect. The first step is to identify a transition between two state of the ion, from now on the associated frequency will be ω_0 . The ion is then irradiated with two laser beam, propagating in opposite direction, with frequency $\omega_{ab} = \omega_0 - \delta\omega$, which is slightly lower than ω_0 ($\delta\omega > 0$). When the ion is in motion with a specific velocity $\mathbf{v}$, it will perceive the laser frequency as exactly ω_0 due to the Doppler effect. When this happens, the ion absorbs a photon and is promoted to the excited state. The chosen excited state is unstable, so the ion re-emits a photon in a random direction and returns to the ground state. The transition is chosen in such a way that its line-width Γ_e associated is much larger than the frequency ω_z and it can be shown that the temperature the ion reaches is given by

$$k_B T \simeq \hbar\Gamma_e. \quad (1.37)$$

To better understand the absorption process, we can write the semiclassical energy and momentum conservation equations

$$\hbar\omega_0 + \frac{1}{2}Mv'^2 = \hbar\omega_{ab} + \frac{1}{2}Mv^2 \quad (1.38)$$

$$M\mathbf{v}' = M\mathbf{v} + \hbar\mathbf{k} \quad (1.39)$$

where $\mathbf{v}'$ is the velocity of the ion just after the absorption and $\mathbf{k}$ is the absorbed photon wave vector. Substituting $\mathbf{v}'$ into the first equation we have

$$\omega_0 = \omega_{ab} - \mathbf{v} \cdot \mathbf{k} - \frac{\hbar^2 k^2}{2M} \quad (1.40)$$

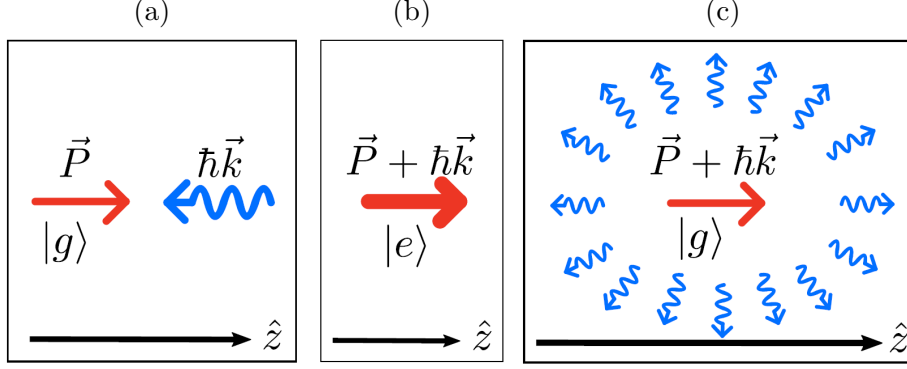


Figure 1.3: Doppler cooling process, (a) and (b): an ion absorbs a red-shifted laser coming towards it and (c) emits it in a random direction. Image taken from [86].

where the second term is the Doppler shift, and the third term is known as the recoil shift [96]. The recoil shift is usually small compared to the Doppler shift at high velocities, we can neglect it and we get

$$\omega_{ab} = \omega_0 + \mathbf{v} \cdot \mathbf{k}. \quad (1.41)$$

Since $\omega_{ab} < \omega_0$, the absorption occurs only if $\mathbf{v} \cdot \mathbf{k} < 0$, and so when $\mathbf{v}$ and $\mathbf{k}$ are opposite directions. We can now consider the emission process. As said before, the excited ion emits a photon in a random direction. In this case the energy and momentum conservation yields to

$$\omega_0 = \omega_{em} - \mathbf{v}' \cdot \mathbf{k}_{em} + \frac{\hbar^2 k^2}{2M} \quad (1.42)$$

where $\mathbf{k}_{em}$ is the emitted photon wave vector and in modulus we have $k_{em} = k$. Neglecting again the recoil shift we have

$$\omega_{em} = \omega_0 + \mathbf{v}' \cdot \mathbf{k}_{em}. \quad (1.43)$$

However, in this phase the photon is emitted in a random direction, therefore, averaging over a great number of scattering processes, we get

$$\langle \hbar \mathbf{v}' \cdot \mathbf{k}_{em} \rangle = 0 \quad (1.44)$$

and so the loss of the ion's kinetic energy is

$$\Delta E_K = -\langle \hbar \Delta \omega \rangle = -\langle \hbar (\omega_{em} - \omega_{ab}) \rangle = \hbar \mathbf{v} \cdot \mathbf{k} < 0. \quad (1.45)$$

In this process (reported schematically in Fig. 1.3), the ion's velocity decreases. Therefore, if we interpret temperature as $\frac{3}{2}k_B T = E_K$, this loss of kinetic energy leads to an effective cooling of the ions. However, ions cannot be cooled indefinitely with this method. Indeed, when the ions are significantly cooled, the recoil term becomes non-negligible, limiting a further slowing down of the ions. Taking into account this term, the change in the ions kinetic energy becomes

$$\Delta E_K = \hbar \mathbf{v} \cdot \mathbf{k} + \frac{\hbar^2 k^2}{M}. \quad (1.46)$$

The ion can continue to cool as long as $\Delta E_K < 0$, which means $-\hbar \mathbf{v} \cdot \mathbf{k} > \frac{\hbar^2 k^2}{M}$ where $\hbar \mathbf{v} \cdot \mathbf{k} > 0$. Using Doppler cooling, temperatures as low as 10^{-6} K can be achieved. Since this is a stochastic process, we must continuously select only the ions that have sufficiently reduced their velocity. As a result, many ions are lost, but the desired temperature can be reached. Notably, with this system, we can cool the ions without the need to cool all the surrounding environment.

1.2.2 Rydberg atoms

Another promising approach to realize natural qubit is given by neutral atoms in the Rydberg state. This method shares many features with trapped ions: qubits result to be intrinsically identical, they have long dephasing time in atomic hyperfine states, and allow manipulation and measurement of qubits state using resonant laser pulses [56]. However, they also exhibit very peculiar properties. Thank to their high principal quantum number n , they have large electric dipole moments. These feature lead to strong interactions with macroscopic external fields or microscopic electromagnetic fields from nearby particles, making systems of Rydberg atoms easier to control [58]. Additionally, these strong interactions can be exploited to induce an effective strong interaction between individual photons, opening up possibilities for performing photonic quantum computation and quantum simulation in a deterministic manner.

In order to describe how it is possible to realize qubit exploiting Rydberg state, it is necessary to show their main properties.

Research in the field of Rydberg atoms starts when, in 1885, Johann Balmer discovered the following formula that describe a series of spectral lines in hydrogen atoms

$$\frac{1}{\lambda} = \frac{1}{B} \left(1 - \frac{4}{m^2} \right) \quad (1.47)$$

where λ is the wavelength, $B = 364.50682$ nm is a constant and $m \in \mathbb{N}$. After that, in 1888, Johannes Rydberg extended the Balmer formula to a more general result

$$\frac{1}{\lambda} = R_H \left(\frac{1}{m^2} - \frac{1}{n^2} \right) \quad (1.48)$$

where λ is again the wavelength, $R_H = 4/B = 1.097 \cdot 10^7 \text{ m}^{-1}$ is a constant and $m, n \in \mathbb{N}$. Eq. (1.48) is known as Rydberg formula.

Any atom, molecule or semiconductor quantum dot in a state with valance electron in a large principal quantum number n state of several tens to hundreds or even higher, namely with a highly-excited electron, can be modelled as a Rydberg atom. This particular electronic structure, with the valance electrons in large, weakly bound orbits, is the reason behind the unique properties of Rydberg atoms. As a consequence, almost all properties of Rydberg atoms show a characteristic scaling with n . First of all, the distribution of energy levels becomes denser as n increases because the energy difference ΔE between neighbouring Rydberg states scales as n^{-3} . As an example, the energy levels of *Rb* are shown in the Fig. 1.4. Note that when $n \sim 100$ we have $\Delta E \sim \text{GHz}$. The size of Rydberg atoms scales as $\langle r \rangle \propto \mu n^2 a_0$ with a_0 the Bohr radius, and finally the dipole moment of Rydberg atoms also scales as n^2 [58].

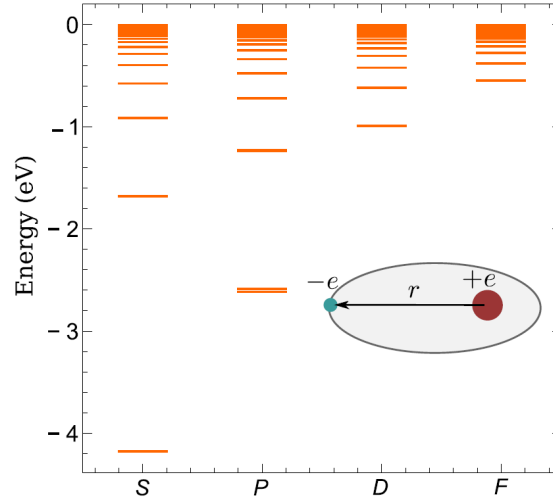


Figure 1.4: Distribution of energy levels for $5 \leq n \leq 60$ of ^{87}Rb atom. Image taken from [58].

One of the properties of Rydberg atoms that makes them more suitable for the realization of qubits is the long lifetime of their excited states. After a characteristic lifetime τ , they decay to their ground state through two main mechanisms: the spontaneous emission and the stimulated emission. The first occurs after an average lifetime τ_0 and is due to vacuum fluctuations of the electromagnetic field at 0 K, while the second is associated to a lifetime τ_{bb} and is caused by blackbody radiation at finite temperature T . As a function of τ_0 and τ_{bb} , the lifetime of a Rydberg atom satisfies the relation [58]

$$\frac{1}{\tau} = \frac{1}{\tau_0} + \frac{1}{\tau_{bb}}. \quad (1.49)$$

The lifetime for spontaneous emission τ_0 for a Rydberg state n is given by

$$\frac{1}{\tau_0} = \sum_{n'} A_{nn'} \quad (1.50)$$

where the sum is calculated over all possible spontaneous emission channels and $A_{nn'}$ is the Einstein coefficient associated to the transition from state n to n' . Using a classical description, if an electron is in a large and so weakly bound orbit, it has a small acceleration and the associated radiation rate is small. As a consequence the lifetime of a Rydberg atom increases with n . Following a more rigorous approach, it is possible to show that $\tau_0 \propto n^3$ for states with low orbital quantum numbers, where the dominant transition is to a low-energy state, and that $\tau_0 \propto n^5$ for states with high orbital quantum numbers, where the dominant transition is to neighbouring Rydberg states. The latter are also called circular Rydberg atoms, and due to the properties just mentioned, they are more suitable for the purpose of realizing qubits.

Stimulated emission due to blackbody radiation also plays a fundamental role in the decay processes of Rydberg atoms. This is the main difference that distinguishes Rydberg atoms from atoms under conventional conditions, where blackbody radiation at room temperature is negligible. The reason behind this difference is the presence of low-frequency transitions with large electric dipole matrix elements that also results in blackbody radiation mainly causing the decay of atoms to nearby Rydberg states. For Rydberg atoms, where n is large, the transitions to focus on

are those with $\omega \ll k_B T$. Their lifetime can be expressed as

$$\tau_{bb} = \frac{3\hbar n^2}{4\alpha_B^3 T} \quad (1.51)$$

where α is the fine structure constant. This means that for Rydberg atoms $\tau_{bb} \propto n^2$. To provide an idea of the time scales involved, the average total lifetime for ^{87}Rb at room temperature, $T = 300$ K and $n \sim 50$ is $\tau \sim 50\mu\text{s}$.

For completeness, it is important to highlight that the two decay mechanisms mentioned above apply only to individual Rydberg atoms. This means that the treatment is valid in experiments with dilute gases, until collective effects become relevant. Due to collective and cooperative effects caused by photon exchange interactions between different Rydberg atoms, the total lifetime decrease in dense gases. In this case, the phenomenon of superradiance also comes into play, photons emitted by excited atoms can cause stimulated emission in other atoms, leading to an avalanche of collective decays [97, 98].

Another relevant feature that makes Rydberg atoms particularly promising for the realization of qubits is that they are characterized by a strong dipole-dipole interaction. The dipole-dipole interaction can be written as

$$V_{dd} = \frac{e^2}{4\pi\epsilon_0} \frac{\mathbf{d}_1 \cdot \mathbf{d}_2 - 3(\mathbf{d}_1 \cdot \mathbf{e}_R)(\mathbf{d}_2 \cdot \mathbf{e}_R)}{R^3} \quad (1.52)$$

where $\mathbf{e}_R$ is the unit vector along the relative coordinate $\mathbf{R}$ between the two atoms and $\mathbf{d}$ is the displacement from the cation to the Rydberg electron. This formula considers the Rydberg atom as an electron dipole composed of its highly excited electron and its cation core with associated dipole moment is $\mathbf{p} = -e\mathbf{d}$. It can be prove that $p \propto n^2$, and thus we have $V_{dd} \propto n^4$. This interaction can be easily controlled, and it is so very versatile; it can be deactivated simply by returning the atoms to their ground state, and its strength, sign, anisotropy, and spatial dependence can be controlled by choosing appropriate states of the atoms. This leads to the so called Rydberg blockade, the inhibition of the excitation of atoms to the Rydberg state by the presence of a nearby Rydberg atom [99]. Considering an atom with ground state $|g\rangle$ and a Rydberg state $|r\rangle$, these two state can be coupled with a resonant laser characterized by a Rabi frequency equal to Ω_R . We can then consider two atoms with a collective ground state $|gg\rangle$, as shown in Fig. 1.5, which is still resonantly coupled to the state $|gr\rangle$ and $|rg\rangle$, characterized by a single Rydberg excitation. Instead, the state $|rr\rangle$, with two Rydberg excitation, is shifted out of resonance by the strong van der Waals interaction U_{vdW} between the two atoms. As long as $U_{vdW} \gg \hbar\Omega_R$ the double excitation is energetically forbidden. The Rydberg blockade was proposed in [100] as a way to implement quantum gates using with neutral atoms.

1.2.3 Superconducting quantum circuits

One of the most common architectures used to experimentally realize artificial qubits is given by superconducting circuits. They are largely exploited in quantum computation and their performances are progressively improving, in particular for what it concerns their decoherence and dephasing times.

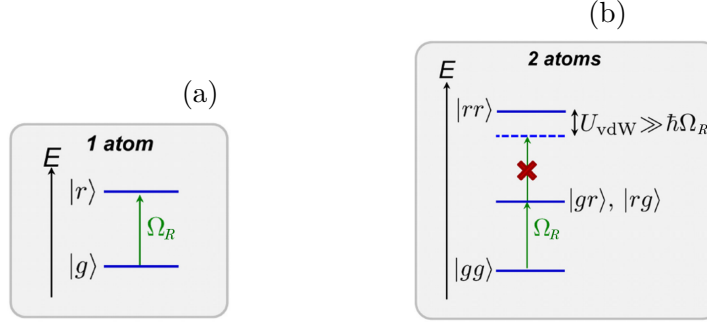


Figure 1.5: Schematic representation of the Rydberg blockade. (a) Atom with ground state $|g\rangle$ and a Rydberg state $|r\rangle$. The two states are coupled with a resonant laser with a Rabi frequency equal to Ω_R . (b) Two atoms with a collective ground state $|gg\rangle$ are still coupled to the states $|gr\rangle$ and $|rg\rangle$. The state $|rr\rangle$ is shifted out of resonance by the strong van der Waals interaction U_{vdW} between the two atoms. Image taken from [99] with minor modifications.

LC circuit

The first element useful to describe the functioning of superconducting qubits is the LC circuit, which can be mapped into a quantum harmonic oscillator. We can therefore consider a circuit made by an inductance L and a capacitance C , as shown in Fig. 1.6, neglecting any resistance since our goal is to describe superconductors, which are naturally dissipationless.

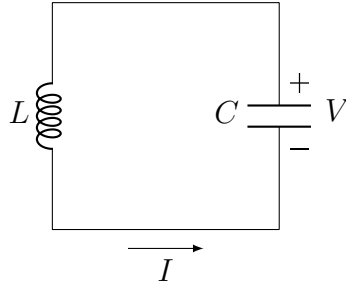


Figure 1.6: Scheme of an LC circuit composed by a capacitance C and an inductance L . I is the current flowing in the circuit and V is the potential difference across the capacitance.

The Lagrangian of the system is given by [78]

$$\mathcal{L} = \frac{1}{2}LI^2 - \frac{1}{2}\frac{Q^2}{C} \quad (1.53)$$

where I is the current in the inductance and Q the charge stored in the capacitance. Using the charge conservation law, $I = \dot{Q}$, we can rewrite the above equation as

$$\mathcal{L} = \frac{1}{2}\dot{Q}^2 - \frac{1}{2}\frac{Q^2}{C}. \quad (1.54)$$

In the following, we will show that this Lagrangian is formally equivalent to that of a harmonic oscillator. To do this, it is convenient to draw a parallel between

the magnetic flux through the inductance, $\Phi(t) = \int_{-\infty}^t d\tau V(\tau)$ ($V = -\frac{Q}{C}$), and the electric charge, Q and the position and its conjugate momentum, typical quantities in the dynamics of systems. This leads to the following equation

$$\Phi = \frac{\delta \mathcal{L}}{\delta \dot{Q}} = L\dot{Q} = LI \quad (1.55)$$

and to the Hamiltonian of the system

$$H = \Phi\dot{Q} - \mathcal{L} = \frac{\Phi^2}{2L} + \frac{1}{2} \frac{Q^2}{C}. \quad (1.56)$$

Finally, we can derive the Hamilton's equations to describe the time evolution of the system [78]

$$\dot{\Phi} = \frac{\partial H}{\partial Q} = \frac{Q}{C} \quad (1.57)$$

$$\dot{Q} = -\frac{\partial H}{\partial \Phi} = -\frac{\Phi}{L}. \quad (1.58)$$

We can now go on with the quantum description of the system. To achieve this, the flux and charge must be promoted to canonically conjugate quantum operators that obey to the commutation relation $[\hat{\Phi}, \hat{Q}] = i\hbar$. Using the following map

$$\begin{cases} C \rightarrow m \\ \frac{1}{L} \rightarrow k \\ \hat{\Phi} \rightarrow \hat{x} \\ \hat{Q} \rightarrow \hat{p}, \end{cases} \quad (1.59)$$

we can describe this system as a quantum harmonic oscillator, where m is the mass, k is the elastic constant of the harmonic oscillator and $\hat{x}$ and $\hat{p}$ are respectively the position and its conjugate momentum. To arrive at the most common form of the quantum harmonic oscillator Hamiltonian, we must introduce creation and annihilation operators, $\hat{a}$ and $\hat{a}^\dagger$, such that $[\hat{a}, \hat{a}^\dagger] = \mathbb{I}$ and related to the previous introduced conjugated operators by [50]

$$\hat{\Phi} = \sqrt{\frac{L}{2\Omega_{LC}}}(\hat{a}^\dagger + \hat{a}) \quad \hat{Q} = i\sqrt{\frac{\Omega_{LC}}{2L}}(\hat{a}^\dagger - \hat{a}) \quad (1.60)$$

with $\Omega_{LC} = \frac{1}{\sqrt{LC}}$. The quantum Hamiltonian can then be rewritten as

$$\hat{\mathcal{H}} = \hbar\Omega_{LC} \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right). \quad (1.61)$$

Before moving on with the description of quantum LC circuit, it is important to recall that for a system to be in the quantum regime, it is necessary to fulfill the condition $k_B T \ll \hbar\Omega_{LC}$ [51]. For this Hamiltonian the eigenvalues of the energy are

$$E_n = \hbar\Omega_{LC} \left(n + \frac{1}{2} \right), \text{ with } n \in \mathbb{N}. \quad (1.62)$$

These energy levels are equidistant, this means that it is not possible to isolate a TLS within them. To realize a TLS, it is crucial to introduce at least a non-linear element in the circuit; in the context of superconducting qubits, this element is the *Josephson junction*.

Josephson junction

To describe how a JJ works, it is necessary to begin with a brief description of the superconducting state of a metal. The main physical effects that occur near the metal-superconductor phase transition can be described using the phenomenological theory of second-order phase transitions developed by Ginzburg-Landau [101]. To describe the superconducting phase in the Ginzburg-Landau theory, a macroscopic order parameter, indicated with ψ , is introduced, which characterizes the transition from the metallic phase, at $T > T_C$, to the superconducting phase, at $T < T_C$. It is assumed that the order parameter ψ , for $T < T_C$, can be interpreted, within the microscopic picture developed later, as being related to the number of Cooper pairs present in the superconductor through the following relation

$$n_{pair}(\mathbf{r}) = |\psi(\mathbf{r})|^2. \quad (1.63)$$

This allows the order parameter to be interpreted as the macroscopic wave function of the Cooper pairs present in the superconducting phase [102].

The Ginzburg-Landau theory is based on the assumption that the free energy density, $f_S(T, \psi)$, near the phase transition takes the following form [101]

$$f_S(T, \psi) = f_N(T) + \alpha(T)|\psi|^2 + \frac{1}{2}\beta(T)|\psi|^4 + \frac{1}{2m^*} \left| \left(\mathbf{p} - \frac{e^*}{c} \mathbf{A} \right) \psi(\mathbf{r}) \right|^2 \quad (1.64)$$

where $f_N(T)$ is the free energy density in the metallic phase. The parameters $\alpha(T)$ and $\beta(T)$ are determined through phenomenological observations

$$\alpha(T) = \alpha_0(T - T_C) \quad \text{with } \alpha_0 > 0 \text{ for } T \sim T_C \quad (1.65)$$

$$\beta(T) = \beta_0 \quad \text{with } \beta_0 > 0 \text{ for } T \sim T_C. \quad (1.66)$$

From the comparison with the microscopic BCS theory, which describes the superconducting phase in terms of Cooper pairs, we identify $m^* = 2m_e$ and $e^* = -2e$, where e is the absolute value of the electron charge. By minimizing Eq. (1.64) with respect to the order parameter, we find that ψ must satisfy the following equation

$$\beta(T)|\psi(\mathbf{r})|^2\psi(\mathbf{r}) + \frac{1}{2m^*} \left(\mathbf{p} - \frac{e^*}{c} \mathbf{A} \right) \psi(\mathbf{r}) = -\alpha(T)\psi(\mathbf{r}). \quad (1.67)$$

It is also possible to write an equation for the supercurrent

$$\mathbf{J}_S(\mathbf{r}) = -i \frac{\hbar e^*}{2m^*} [\psi^*(\mathbf{r}) \nabla \psi(\mathbf{r}) - \psi(\mathbf{r}) \nabla \psi^*(\mathbf{r})] - \frac{e^{*2}}{m^* c} |\psi(\mathbf{r})|^2 \mathbf{A}(\mathbf{r}). \quad (1.68)$$

By expressing the order parameter in polar coordinates, $\psi(\mathbf{r}) = |\psi(\mathbf{r})| e^{i\theta(\mathbf{r})}$, Eq. (1.68) can be rewritten as

$$\mathbf{J}_S(\mathbf{r}) = |\psi(\mathbf{r})|^2 \left(\frac{\hbar e^*}{m^*} \nabla \theta(\mathbf{r}) - \frac{e^{*2}}{m^* c} \mathbf{A}(\mathbf{r}) \right). \quad (1.69)$$

Now we can consider a superconducting ring as shown in Fig. 1.7. Due to the Meissner effect [102], inside the superconductor we have

$$\mathbf{J}_S(\mathbf{r}) = 0. \quad (1.70)$$

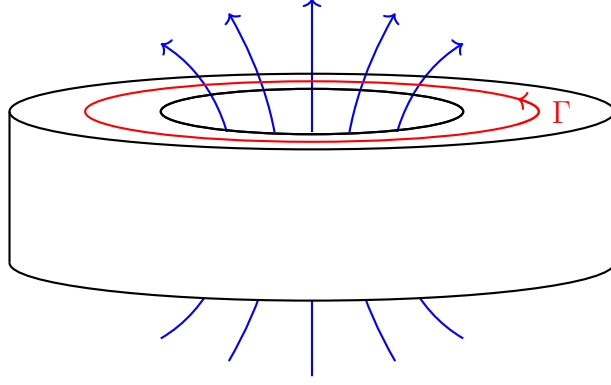


Figure 1.7: Flux quantization through a superconducting ring.

and substituting into Eq. (1.69) we obtain

$$\nabla\theta(\mathbf{r}) = \frac{e^*}{\hbar c} \mathbf{A}(\mathbf{r}). \quad (1.71)$$

Integrating Eq. (1.71) over a closed path Γ (red line in Fig. 1.7) inside the superconductor yields

$$\oint_{\Gamma} \nabla\theta(\mathbf{r}) \cdot d\mathbf{l} = \frac{e^*}{\hbar c} \oint_{\Gamma} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{l} = \frac{e^*}{\hbar c} \iint_{\mathcal{S}} \nabla \times \mathbf{A}(\mathbf{r}) \cdot d\mathbf{S}. \quad (1.72)$$

In the second step, Stokes' theorem has been applied, with $\mathcal{S}$ being the surface bounded by the curve Γ . According to the gradient theorem, given a curve Γ oriented from a point $\mathbf{p}$ to a point $\mathbf{q}$, we have

$$\Delta\theta \equiv \theta(\mathbf{q}) - \theta(\mathbf{p}) = \int_{\mathbf{p},\Gamma}^{\mathbf{q}} \nabla\theta(\mathbf{r}) \cdot d\mathbf{l}. \quad (1.73)$$

The left-hand side of Eq. (1.72) therefore represents the variation $\Delta\theta$ along the closed path Γ . From the definition of the vector potential $\mathbf{A}$, we have

$$\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r}). \quad (1.74)$$

The right-hand side of Eq. (1.72) thus contains the magnetic field flux $\Phi(\mathbf{B})$ through the surface $\mathcal{S}$

$$\Phi(\mathbf{B}) = \iint_{\mathcal{S}} \mathbf{B}(\mathbf{r}) \cdot d\mathbf{S}. \quad (1.75)$$

Substituting Eqs. (1.73) and (1.75) into (1.72), we obtain

$$\Phi(\mathbf{B}) = \frac{\hbar c}{e^*} \Delta\theta. \quad (1.76)$$

Since θ is a phase, its variation along a closed path must be an integer multiple of 2π : $\Delta\theta = 2\pi n$, with $n \in \mathbb{Z}$. This observation leads to the quantization of the flux $\Phi(\mathbf{B})$

$$\Phi(\mathbf{B}) = \frac{\hbar c}{2e} n \equiv \Phi_0 n \quad (1.77)$$

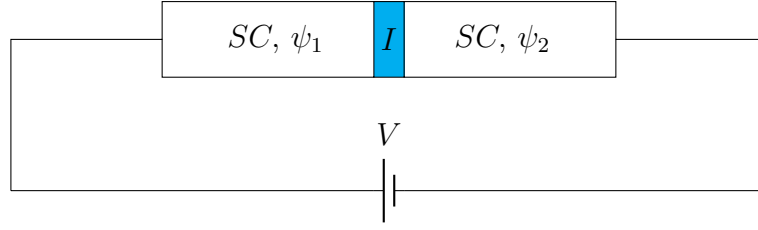


Figure 1.8: Schematic representation of a JJ connected to a battery with potential difference V . The blue region represent the thin layer of insulating material.

where $\Phi_0 = \frac{hc}{2e}$ is defined as the *elementary quantum flux*. At this point, it is possible to consider a JJ consisting of two layers of superconducting material separated by a thin layer of insulating material, as shown in Fig. 1.8. If the insulating material were infinitely thick, the two superconducting materials would be decoupled and thus described by two distinct order parameters

$$\psi_1 = |\psi_1| e^{i\theta_1} \quad \text{and} \quad \psi_2 = |\psi_2| e^{i\theta_2} \quad (1.78)$$

with $|\psi_{1/2}|$ and $\theta_{1/2}$ uniform within superconductors 1 and 2, respectively.

However, if the two superconductors are separated by a barrier of thickness b , it is expected that the order parameters decay exponentially within the insulating region. Therefore, it becomes possible to describe the system using a single order parameter

$$\psi(z) = \psi_1 e^{-\lambda z} + \psi_2 e^{-\lambda(z-b)}. \quad (1.79)$$

With λ as the parameter characterizing the decay in the insulating region and z as the axis perpendicular to the interfaces between the different materials, the origin of the z -axis is placed at the interface between the first superconducting layer and the insulating barrier. By substituting into Eq. (1.69), in the absence of a magnetic field, one obtains

$$J_S(z) = \frac{2\hbar e^*}{2m^*} \beta e^{-\lambda b} |\psi_1| |\psi_2| \sin(\theta_2 - \theta_1). \quad (1.80)$$

It is important to note that the supercurrent between the two superconductors is proportional to the phase difference between the order parameters of the two superconductors. Defining $\varphi = \theta_2 - \theta_1$ and I_J as the current determined by the geometric and physical properties of the junction, we have

$$I = I_J \sin \varphi. \quad (1.81)$$

In the presence of a potential difference V between the two superconductors, there is an energy difference equal to $2eV$ between the Cooper pairs of one superconductor relative to the other. Recalling the interpretation of ψ as a wave function, it is possible to write the Schrödinger equations for ψ_1 and ψ_2 as [63, 103, 104]

$$i\hbar \frac{d\psi_1}{dt} = -eV\psi_1 + K\psi_2 \quad (1.82)$$

$$i\hbar \frac{d\psi_2}{dt} = eV\psi_2 + K\psi_1 \quad (1.83)$$

with K the tunnelling amplitude between the two superconductors [104]. Substituting the expression of ψ_1 and ψ_2 in polar coordinates into Eqs. (1.82) and (1.83)

and considering only the imaginary part, we arrive at the following equations

$$\frac{d\theta_1}{dt} = -\frac{K}{\hbar} \sqrt{\frac{|\psi_2|}{|\psi_1|}} \cos \theta + \frac{eV}{\hbar} \quad (1.84)$$

$$\frac{d\theta_2}{dt} = -\frac{K}{\hbar} \sqrt{\frac{|\psi_1|}{|\psi_2|}} \cos \theta - \frac{eV}{\hbar}. \quad (1.85)$$

If we assume two identical superconductors, we have $|\psi_1| \sim |\psi_2|$, and therefore we obtain

$$\frac{d\varphi}{dt} = \frac{d\theta_2}{dt} - \frac{d\theta_1}{dt} = \frac{2eV}{\hbar}. \quad (1.86)$$

Eqs. (1.81) and (1.86) are called the *first* and *second Josephson equations*, respectively [104]. By differentiating the first Josephson equation, we get

$$\dot{I} = I_J \cos \varphi \frac{d\varphi}{dt} \quad (1.87)$$

and recalling that $\dot{I} = \frac{V}{L}$, we obtain the expression for a nonlinear inductance

$$L_J = \frac{1}{\cos \varphi} \frac{\Phi_0}{2\pi I_J}. \quad (1.88)$$

The electromagnetic energy stored in such a circuit element is

$$E_{J,L} = \int_0^t I(\tau) V d\tau = E_J (1 - \cos \varphi) \quad (1.89)$$

with $E_J = \frac{\Phi_0 I_J}{2\pi}$ being the characteristic energy of the JJ. The junction also has a capacitance C_J , this leads to the additional energy contribution

$$E_{J,C} = \frac{Q^2}{2C_J} \quad (1.90)$$

where Q is the charge stored within the junction. If N_1 and N_2 are the number of Cooper pairs in the two superconducting layers respectively, we define $N = N_1 - N_2$ as the *excess* of Cooper pairs in the junction. The charge in the junction is therefore $2eN$. Based on previous reasoning, the classical Hamiltonian associated with a JJ can be written as

$$H_J = \frac{Q^2}{2C_J} - E_J \cos \varphi = 4E_C N^2 - E_J \cos \varphi \quad (1.91)$$

where $E_C = \frac{e^2}{2C_J}$ and the constant term has been neglected. By associating the term $4E_C N^2$ with kinetic energy and $-E_J \cos \varphi$ with potential energy, the Hamiltonian of a JJ corresponds to that of an anharmonic oscillator, where the conjugate variables are

$$\varphi \in (0, 2\pi) \rightarrow x \quad N \in (-\infty, +\infty) \rightarrow p. \quad (1.92)$$

It should be noted that the identification made here is the same made in Section 1.2.3 for the LC oscillator. At this point, it is possible to promote φ and N to operators

that satisfy a canonical commutation relation $[\hat{\varphi}, \hat{N}] = i$, and write the quantum Hamiltonian in the form

$$\hat{\mathcal{H}}_J = 4E_C \hat{N}^2 - E_J \cos \hat{\varphi}. \quad (1.93)$$

It is useful to note that while it can be solved in general for arbitrary ratios between the parameters E_J and E_C [76], it is more insightful to distinguish between different configurations based on their limiting behavior. In the following, we will analyze the charge qubit with $E_C \gg E_J$, and the flux and transmon qubit if instead $E_C \ll E_J$ [77, 78]. The latter is the configuration used in IBM's quantum computers.

Charge qubit

The first example of qubit that we analyze works in the regime where $E_J \ll E_C$. It is called charge qubit or *Cooper pair box* [52, 53]. In this configuration, the JJ is connected to a gate voltage V_g through a gate capacitance C_g as represented in Fig. 1.9.

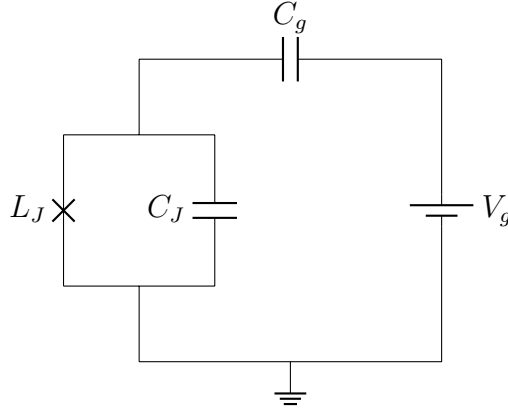


Figure 1.9: Scheme of a charge qubit. Here the JJ, characterized by a capacitance C_J and an inductance L_J , is coupled to an external voltage V_g via an external capacitance C_g .

The presence of V_g introduces a shift in the value of N equal to a quantity $N_g = \frac{C_g V_g}{2e}$, allowing control of the junction — and thus the qubit — from the outside. Recalling Eq. (1.93), the Hamiltonian can be rewritten as

$$H_J = 4E_C (\hat{N} - N_g)^2 - E_J \cos \hat{\varphi}, \quad (1.94)$$

with $E_C = \frac{e^2}{2(C_J + C_g)}$ redefined accordingly.

To identify two energy states that can be used as a qubit, it is convenient to rewrite the Hamiltonian in the basis of eigenstates $|N\rangle$, states with a defined number of Cooper pairs [53]

$$\hat{N} |N\rangle = N |N\rangle. \quad (1.95)$$

From this basis, one can also construct the basis of eigenstates of $\hat{\varphi}$

$$|\varphi\rangle = \sum_{N=-\infty}^{\infty} e^{iN\varphi} |N\rangle \quad (1.96)$$

and the inverse relation

$$|N\rangle = \frac{1}{2\pi} \int_0^{2\pi} e^{-iN\varphi} |\varphi\rangle d\varphi. \quad (1.97)$$

It is also useful to define the operator $e^{i\hat{\varphi}}$

$$e^{i\hat{\varphi}} = \frac{1}{2\pi} \int_0^{2\pi} e^{i\varphi'} |\varphi'\rangle \langle \varphi'| d\varphi'. \quad (1.98)$$

By direct calculation, one verifies that

$$e^{i\hat{\varphi}} |\varphi\rangle = e^{i\varphi} |\varphi\rangle \quad (1.99)$$

$$e^{i\hat{\varphi}} |N\rangle = |N-1\rangle. \quad (1.100)$$

Since Eq. (1.100) holds for all $|N\rangle$, we have

$$e^{i\hat{\varphi}} = \sum_N |N-1\rangle \langle N| \quad e^{-i\hat{\varphi}} = \sum_N |N\rangle \langle N-1|. \quad (1.101)$$

This allows us to rewrite Hamiltonian in Eq. (1.93) in terms of the basis $\{|N\rangle\}$

$$\begin{aligned} \hat{\mathcal{H}}_J &= 4E_C(\hat{N} - N_g)^2 - E_J \cos \hat{\varphi} = 4E_C(\hat{N} - N_g)^2 - \frac{1}{2}E_J(e^{i\hat{\varphi}} + e^{-i\hat{\varphi}}) = \\ &= \sum_{N=-\infty}^{+\infty} \left[4E_C(N - N_g)^2 |N\rangle \langle N| - \frac{1}{2}E_J(|N-1\rangle \langle N| + |N\rangle \langle N-1|) \right]. \end{aligned} \quad (1.102)$$

The second term in the Hamiltonian, $|N-1\rangle \langle N| + |N\rangle \langle N-1|$, describes the tunnelling of one Cooper pair through the junction because it changes the difference N by one unit at a time. E_J can be seen then as the amplitude of the tunnelling across the junction. Thanks to the limit $E_J \ll E_C$, it is possible to deal with this term using a perturbative approach. The unperturbed Hamiltonian

$$\hat{\mathcal{H}}_{J0} = 4E_C \sum_{N=-\infty}^{+\infty} (N - N_g)^2 |N\rangle \langle N| \quad (1.103)$$

is diagonal in the basis $\{|N\rangle\}$ with eigenvalues

$$E_{J0}(N, N_g) = 4E_C(N - N_g)^2. \quad (1.104)$$

In Fig. 1.10 are shown the energy levels for different value of N , as a function of N_g . There are two degeneracy points at $N = \pm \frac{1}{2}$, and the same behavior would have been observed for any $N = N_g - \frac{1}{2}$, due to the periodicity in the Hamiltonian. The aim of the last part of this Paragraph is to show that such degeneracy is broken by the addition of the perturbative term in the Hamiltonian

$$\hat{\mathcal{H}}_{J1} = -\frac{E_J}{2} \sum_{N=-\infty}^{+\infty} (|N-1\rangle \langle N| + |N\rangle \langle N-1|). \quad (1.105)$$

Thank to the periodicity in N_g , Fig. 1.11, and without loss of generality, we can focus on $N = 0$. For $E_J \ll E_C$, only the levels $|N\rangle$ and $|N-1\rangle$ are coupled by the

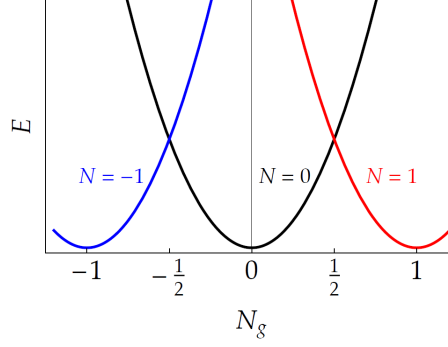


Figure 1.10: Energy levels of $\hat{\mathcal{H}}_{J0}$ for $N = -1, 0, 1$ as a function of N_g . Image taken from [52].

perturbative Hamiltonian $\hat{\mathcal{H}}_{J1}$. To simplify the notation, we can introduce Δ_g such that $N_g = N + \frac{1}{2} + \Delta_g$. Under these assumption the Hamiltonian becomes

$$\begin{aligned}
 \hat{\mathcal{H}}_{ch} &= 4E_C \left[\left(\frac{1}{2} + \Delta_g \right)^2 |0\rangle\langle 0| + \left(\frac{1}{2} - \Delta_g \right)^2 |1\rangle\langle 1| \right] - \frac{E_J}{2} (|0\rangle\langle 1| + |1\rangle\langle 0|) \\
 &= 4E_C \left(\frac{1}{4} + \Delta_g^2 \right) (|0\rangle\langle 0| + |1\rangle\langle 1|) + 4E_C \Delta_g (|0\rangle\langle 0| - |1\rangle\langle 1|) - \\
 &\quad - \frac{E_J}{2} (|0\rangle\langle 1| + |1\rangle\langle 0|) \\
 &= 4E_C \left(\frac{1}{4} + \Delta_g^2 \right) \mathbb{I} + 4E_C \Delta_g \hat{\sigma}_z - \frac{E_J}{2} \hat{\sigma}_x.
 \end{aligned} \tag{1.106}$$

The eigenvalues of this Hamiltonian are

$$E_{\pm} = 4E_C \left(\frac{1}{4} + \Delta_g^2 \right) \pm \frac{E_J}{2} \sqrt{1 + \frac{64E_C^2 \Delta_g^2}{E_J^2}} \tag{1.107}$$

and, as shown in Fig. 1.11, they are no more degenerate. From Eq. (1.107), it is

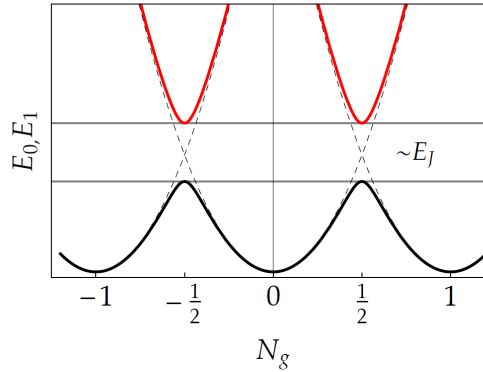


Figure 1.11: Energy levels for different value of N , as a function of N_g with $E_J \ll E_C$. Image taken from [52].

possible to evaluate the amplitude of the gap opened by the Josephson term

$$\Delta E \equiv E_+ - E_- = E_J \sqrt{1 + \frac{64E_C^2 \Delta_g^2}{E_J^2}} \tag{1.108}$$

and identify two limit regimes

$$\begin{cases} \Delta E \simeq E_J & \text{if } \frac{64E_C^2\Delta_g^2}{E_J^2} \ll 1 \\ \Delta E \simeq 2E_C\Delta_g & \text{if } \frac{64E_C^2\Delta_g^2}{E_J^2} \gg 1. \end{cases} \quad (1.109)$$

In the first case, the energy gap is independent of N_g , which implies that the Cooper pair box is protected from noise due to fluctuations in N_g . For this reason, the point $\Delta_g = 0$ is commonly referred to as the sweet spot. This indicates that the coupling has a significant effect only near the degeneracy point. Therefore, we can identify $\frac{64E_C^2\Delta_g^2}{E_J^2} \simeq 1$ as the boundary of the region where the correction due to the Josephson term is relevant. By substituting the definition of Δ_g , we obtain

$$\Delta_g \simeq \frac{E_J}{8E_C}. \quad (1.110)$$

This expression makes it clearer that the amplitude of the energy gap is governed by the ratio between E_J and E_C , thereby justifying the approximation used. It has been observed that the energy gap between the states $|0\rangle$ and $|1\rangle$ depends on V_g , enabling experimental control over the system's dynamics. However, several factors cannot be controlled experimentally, leading to fluctuations in V_g and introducing noise into the system. The superconducting island of a Cooper pair box must be sufficiently small so that the addition of a single Cooper pair results in a significant energy change. As a result, the Cooper pair box is highly sensitive to variations in its surrounding environment. This phenomenon is commonly referred to as charge noise. To address these challenges, it is often preferable to operate in the opposite regime, which will be discussed in the following Paragraphs.

Flux qubit

This Paragraph is dedicated to the opposite limit with respect to the charge qubit, namely $E_J \gg E_C$. Due to the degree of freedom used to control it, a qubit working in this regime is indicated as flux qubit [53]. The limit $E_J \gg E_C$ allows us to neglect the charge term in the Hamiltonian in Eq. (1.93) and consider this approximate expression

$$H_{fl,J} \simeq -E_J \cos \varphi. \quad (1.111)$$

As shown in Fig. 1.12, to control the system, an external inductance, L , and an external magnetic flux, ϕ_E , are added to the JJ. We can now write the complete Hamiltonian of the circuit in Fig. 1.12. The term associated to the inductance is given by

$$U_L \equiv \frac{\Phi^2}{2L} = \frac{\varphi^2}{8e^2L} \quad (1.112)$$

while the term associated to the external magnetic flux is

$$U_{ext} \equiv -\mathcal{M} \cdot \mathbf{B} = -\frac{\varphi\varphi_e}{4e^2L} \quad (1.113)$$

with $\mathcal{M} = IS$ the magnetic momentum associated to the circuit, S the area of the superconducting circuit, $I = \frac{\Phi}{L}$ the current through the circuit, and $\varphi_e = 2e\phi_E$.

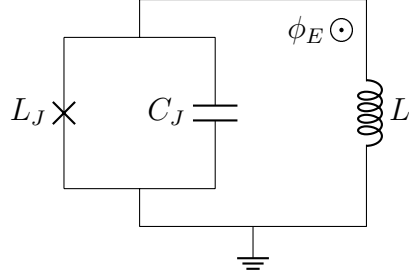


Figure 1.12: Scheme of a flux qubit composed by a JJ, characterized by a capacitance C_J and an inductance L_J , an external inductance L and an external magnetic flux ϕ_E .

Neglecting the constant term, the total energy contribution associated to these two external element is given by

$$U_{\mathcal{F}} \equiv U_L + U_{ext} = E_{\mathcal{F}} \frac{(\varphi - \varphi_e)^2}{2} \quad (1.114)$$

with $E_{\mathcal{F}} = \frac{\hbar^2}{4e^2 L}$. If the inductance is chosen in such a way that $E_J \sim E_{\mathcal{F}}$, we have $4E_C N \ll U_{\mathcal{F}}$. Then, the total Hamiltonian of the flux qubit is

$$H_{fl} \simeq -E_J \cos \varphi + E_{\mathcal{F}} \frac{(\varphi - \varphi_e)^2}{2}. \quad (1.115)$$

Now we have to determine under which condition this system can work as a qubit. In this kind of circuit, this occurs in the regions where the potential is well approximated by a double well potential. From a qualitative point of view, the energy, shown in Fig. 1.13, is given by the sum of a cosine and a parabola and gives anharmonic energy levels. According to this, a double well profile centered in one of the cosine

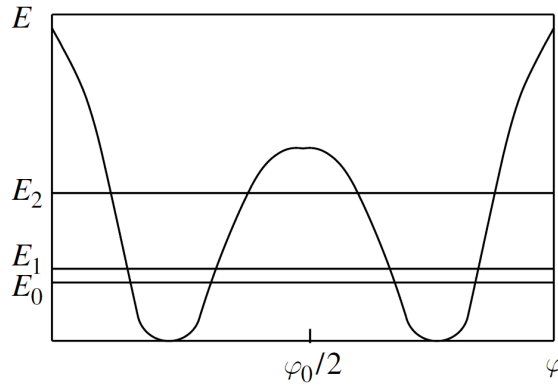


Figure 1.13: Double-well potential of the flux qubit with the first three quantum levels in the wells and $\varphi_e = \varphi_0/2$. Image taken from [51].

maxima can be obtained when $\varphi_e = (2k + 1)\pi$ ($k \in \mathbb{Z}$) and for $E_J \sim E_{\mathcal{F}}$. Without loss of generality, we can focus on the maximum $\varphi = \pi$. Using a perturbative approach, we can Taylor expand the Hamiltonian up to the fourth order in such a way that

$$H_{fl} \simeq E_{\mathcal{F}} \left(-\epsilon \frac{\tilde{\varphi}^2}{2} - f \tilde{\varphi} + \frac{1 + \epsilon}{24} \tilde{\varphi}^4 \right) \quad (1.116)$$

with $\tilde{\varphi} = \varphi - \pi$, $f = \varphi_e - \pi$ and $\epsilon = \frac{E_J}{E_F} - 1 \ll 1$. It is worth to note that, according to the above definitions, we have $f = 0$ for $\varphi_e = \pi$. To identify the two levels that can be used to realize a qubit, it is useful to approximate the double-well potential with two parabolic potentials, U_l and U_r , as shown in Fig. 1.14. We can introduce the corresponding ground state wave function, $|l\rangle$ and $|r\rangle$, such that they satisfy the stationary Schrödinger equation

$$\hat{\mathcal{H}}_l |l\rangle = E_l |l\rangle, \quad \hat{\mathcal{H}}_r |r\rangle = E_r |r\rangle \quad (1.117)$$

with $\hat{\mathcal{H}}_{l/r}$ the Hamiltonian associated to the potential $U_{l/r}$.

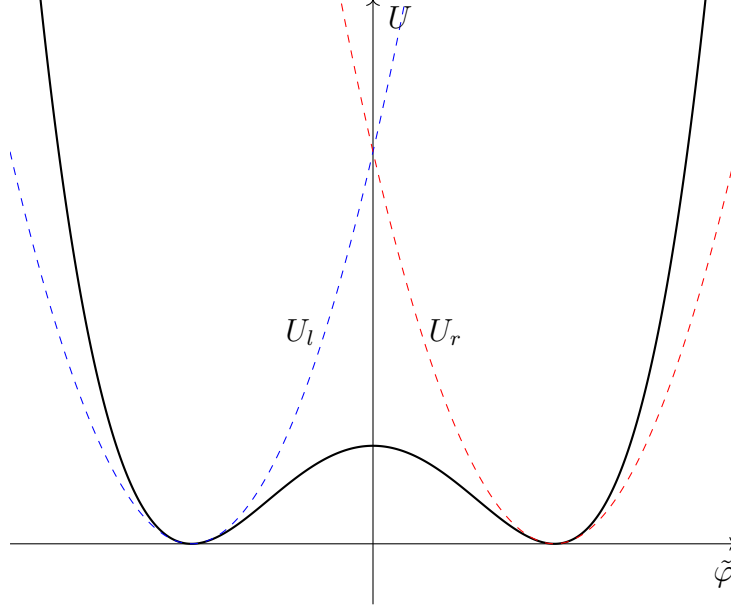


Figure 1.14: Truncation of the flux qubit Hamiltonian; dashed lines indicate potentials of the left and right.

In the two wells, the averaged induced flux have opposite signs. This lead to opposite directions of the circulating persistent currents. The true eigenvectors can so be approximate as

$$\hat{\mathcal{H}} |E\rangle = E |E\rangle \quad (1.118)$$

with $|E\rangle = a |l\rangle + b |r\rangle$. We can now write the matrix elements of the total Hamiltonian $\hat{\mathcal{H}}$

$$H_{ll} \equiv \langle l | \hat{\mathcal{H}} | l \rangle = E_l + \langle l | U - U_l | l \rangle \simeq E_l \quad (1.119)$$

$$H_{rr} \equiv \langle r | \hat{\mathcal{H}} | r \rangle = E_r + \langle r | U - U_r | r \rangle \simeq E_r \quad (1.120)$$

$$H_{rl} \equiv \langle r | \hat{\mathcal{H}} | l \rangle = E_l \langle r | l \rangle + \langle r | U - U_r | l \rangle. \quad (1.121)$$

The diagonal matrix elements can be approximate with $E_{l/r}$ because the wave functions are exponentially small in the region where the deviation of the approximated potential from the true one is appreciable. The off-diagonal matrix element is exponentially small because of small overlap of the ground state wave functions in the left and right wells. Note that the truncated Hamiltonian is symmetric, so $H_{rl} = H_{lr}$. We can rewrite the approximate Hamiltonian of the flux qubit $\hat{\mathcal{H}}$ in a way formally equivalent to the one of the charge qubit, reported in Eq. (1.106),

$$\hat{\mathcal{H}} = -\frac{1}{2}(\epsilon \hat{\sigma}_z + \Delta \hat{\sigma}_x) \quad (1.122)$$

with

$$\epsilon = E_r - E_l \text{ and } \frac{\Delta}{2} = H_{rl}. \quad (1.123)$$

Also the energy spectrum of the flux qubit is the same of the charge qubit in Eq. (1.108),

$$E_{1,2} = \mp \frac{1}{2} \sqrt{\epsilon^2 + \Delta^2} \quad (1.124)$$

but the physical meaning is different. The flux qubit Hamiltonian is written in the flux basis, the basis of the states with certain averaged induced flux, $\phi_{l/r}$, rather than the charge basis of the charge qubit.

Transmon qubit

We now introduce a different type of superconducting qubit that offers improved performance compared to the charge and flux qubits discussed in the previous Paragraphs, and currently represents the state-of-the-art among artificial qubits. In particular, we describe one of the earliest proposals for the so-called transmon qubit (transmission line shunted plasma oscillation qubit) [52, 77]. This qubit was specifically designed to reduce sensitivity to charge noise. The transmon achieves this by adopting a circuit configuration similar to that of the charge qubit, while operating in the same parameter regime as the flux qubit. This is accomplished by introducing a large shunting capacitance C_B in parallel with the JJ, as illustrated in Fig. 1.15. Even though the transmon works in the same regime of the flux qubit it has the advantage of being easier to build and control. In fact it is much more difficult to fine tuning the external magnetic flux to have the optimal working performances of the flux qubit compared to adding the shunted capacitance and gate voltage of the transmon. This external capacitance C_B modifies the charging energy as

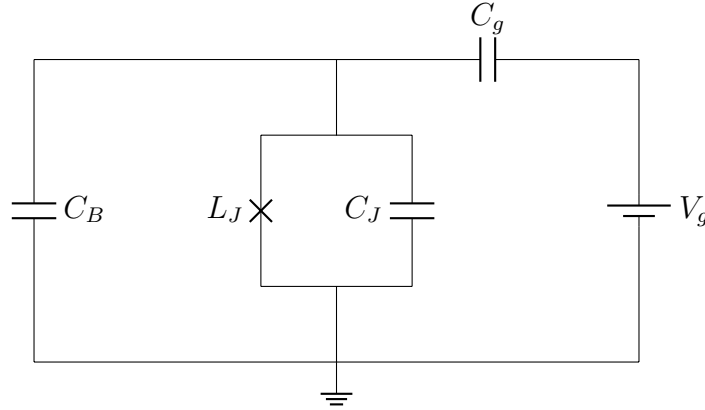


Figure 1.15: Scheme of a transmon qubit. It is analogous to a charge qubit where a large capacitance is added in parallel to reduce the charging energy E_C .

$$E_C = \frac{e^2}{2(C_J + C_g + C_B)} \quad (1.125)$$

reducing its value. If C_B is big enough it is possible to access the regime $E_J \gg E_C$.

As already done for the charge qubit and the flux qubit, we now want to understand how the transmon qubit can operate as a TLS. In the limit $E_J \gg E_C$, it

is possible to expand the cosine term in Eq. (1.93) around one of the minima of $-\cos\varphi$. Without loss of generality, we chose the value $\varphi = 0$ and expand up to fourth order. This leads to the approximated Hamiltonian

$$\hat{\mathcal{H}}_{tr} = 4E_C \hat{N}^2 + \frac{1}{2}E_J \hat{\varphi}^2 - \frac{1}{24}E_J \hat{\varphi}^4. \quad (1.126)$$

The first two terms constitute the Hamiltonian of a harmonic oscillator, while the last term introduces the desired anharmonicity. It is useful to introduce the bosonic creation and annihilation operators $\hat{b}$ and $\hat{b}^\dagger$, such that $[\hat{b}, \hat{b}^\dagger] = \mathbb{I}$. It is possible to write the operators $\hat{N}$ and $\hat{\varphi}$ in terms of the bosonic operators as

$$\hat{\varphi} = 2\sqrt{\frac{E_C}{\hbar\omega_p}}(\hat{b}^\dagger + \hat{b}) \quad (1.127)$$

$$\hat{N} = \frac{i}{4}\sqrt{\frac{\hbar\omega_p}{E_C}}(\hat{b}^\dagger - \hat{b}) \quad (1.128)$$

with $\omega_p = \frac{\sqrt{8E_CE_J}}{\hbar}$ the Josephson frequency. Replacing the relations above into Eq. (1.126) we get

$$\hat{\mathcal{H}}_{tr} = \hbar\omega_p \left(\hat{b}^\dagger \hat{b} + \frac{1}{2} \right) - \frac{1}{12}E_C(\hat{b}^\dagger + \hat{b})^4. \quad (1.129)$$

Recalling the limit $E_C \ll E_J$ and noting that this implies $E_C \ll \hbar\omega_p$, we can evaluate the eigenvalues of this Hamiltonian in a perturbative way. We can define

$$\hat{\mathcal{H}}_{tr}^{(0)} = \hbar\omega_p \left(\hat{b}^\dagger \hat{b} + \frac{1}{2} \right) \quad (1.130)$$

as the unperturbed Hamiltonian with eigenvalues equal to the ones of the harmonic oscillator

$$E_n^{(0)} = \hbar\omega_p \left(n + \frac{1}{2} \right) \quad (1.131)$$

and

$$\hat{\mathcal{H}}_{tr}^{(1)} = -\frac{1}{12}E_C(\hat{b}^\dagger + \hat{b})^4 \quad (1.132)$$

the perturbation term. The first order correction to $E_n^{(0)}$ is given by

$$E_n^{(1)} = -\langle n | \left[\frac{1}{12}E_C(\hat{b}^\dagger + \hat{b})^4 \right] | n \rangle = -E_C n - \frac{1}{2}E_C n(n-1) - \frac{1}{4} \quad (1.133)$$

with $|n\rangle$ the eigenvectors of $\hat{\mathcal{H}}_{tr}^{(0)}$. Up to this perturbative order and neglecting constant terms, the energy levels of the transmon qubit are given by

$$E_n = (\hbar\omega_p - E_C)n - \frac{1}{2}E_C n(n-1). \quad (1.134)$$

The energy difference between two consecutive levels is now a function of n and can be written as

$$\Delta E_{n,n+1} \equiv E_{n+1} - E_n = (\hbar\omega_p - E_C) - E_C n. \quad (1.135)$$

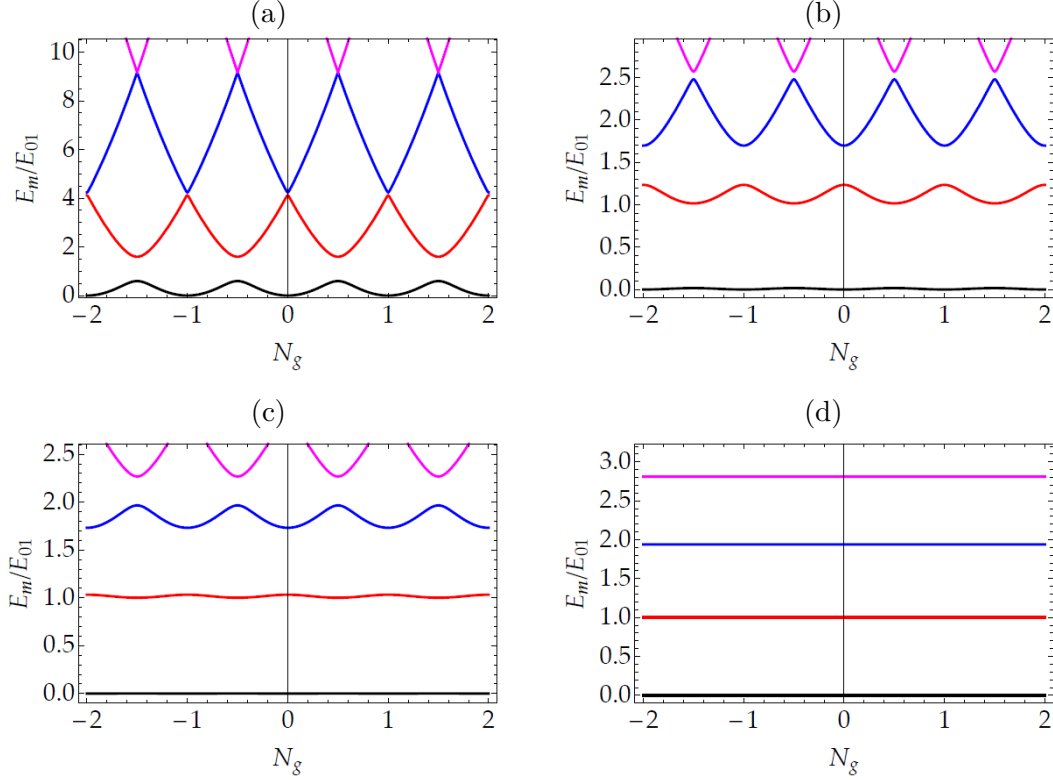


Figure 1.16: The figure shows the first four energy levels (normalized with respect to $E_{01} = \min_{N_g}(E_1 - E_0)$) of the Hamiltonian in Eq. (1.129) for different values of the ratio E_J/E_C . In (a) $E_J/E_C = 1.0$; in (b) $E_J/E_C = 5.0$; in (c) $E_J/E_C = 10.0$; and in (d) $E_J/E_C = 50.0$. Image taken from [52].

Looking at the firsts levels we have

$$\Delta E_{0,1} - \Delta E_{1,2} = E_C. \quad (1.136)$$

Fig. 1.16 represents exact solutions of the system for various parameter regimes; panels (a) and (d) correspond to cases where the perturbative limits discussed earlier also apply. For $\frac{E_J}{E_C} = 10$ we have a good anharmonicity between the levels, but the qubit is still charge sensitive. To achieve sufficiently high anharmonicity and low charge noise, it was demonstrated that the optimal energy ratio for the realization of a transmon must satisfy the following inequality [77]

$$20 \lesssim \frac{E_J}{E_C} \ll 5 \cdot 10^4. \quad (1.137)$$

Summarizing:

- as E_C increases, anharmonicity increases.
- as E_C decreases, with E_J fixed, insensitivity to charge noise increases.

In this operating regime, the transmon qubit exhibits better decoherence and dephasing times compared to other superconducting qubits. These characteristic times can reach approximately $10^2 \mu\text{s}$, which should be compared to the typical duration of a unitary operation, that is around 10 ns for the transmon. This implies

that roughly 10^4 operations can be performed within the coherence time, making the transmon one of the most widely adopted qubit architectures in recent advances in quantum computing, as used for instance by Google and IBM.

Within this regime, if the system is initialized in the state $|0\rangle$ and supplied with energy equal to $\hbar\omega_p$, the only accessible state is $|1\rangle$. This enables the use of the two-level approximation. By neglecting higher excited states, the Hamiltonian in Eq. (1.129) of the system can be expressed in the computational basis as

$$\hat{\mathcal{H}}_{tr} = -\frac{1}{2}\hbar\omega_p\hat{\sigma}_z, \quad (1.138)$$

where we have neglected an additive constant.

1.2.4 Noise and decoherence

Section 1.1 described the main features of an isolated TLS. In particular, Section 1.1.2 discussed the time evolution of a closed system governed by a time-independent Hamiltonian. It was shown that this evolution is fully determined once the initial state and the system's Hamiltonian are known. However, as introduced in Section 1.1.1, it is not always possible to have a complete knowledge of the system. When a qubit interacts with its environment, additional degrees of freedom must be considered, which make the time evolution of the qubit's state no longer fully deterministic. This phenomenon is generally referred to as *noise*, and it can have both systematic and stochastic contributions. Systematic noise can be corrected if its sources are identified. Stochastic noise, on the other hand, arises from random fluctuations in parameters coupled to the qubit and leads to decoherence of the system [105]. Decoherence refers to any process that results in a loss of information about the quantum state of the system [66]. It is associated with uncontrolled interactions between the system and the environment, which lead to the formation of an entangled state. There are two main types of processes that cause decoherence: relaxation and dephasing. Relaxation is an energy-loss process in which the system transfers energy to the environment. When a qubit is in the excited state $|1\rangle$, there is a non-zero probability per unit time that it will spontaneously decay to the ground state $|0\rangle$. This decay usually follows an exponential law and is characterized by the relaxation time T_1 [66]. Dephasing, on the other hand, is a non-dissipative process typically linked to coupling between the qubit's phase and the environment. It results in random phase shifts of the qubit and is characterized by the dephasing time T_2 [66]. In terms of the density operator, an initial state

$$\rho = \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix}, \quad (1.139)$$

which may describe, for instance, a pure system in a superposition state, evolves under dephasing towards

$$\rho \longrightarrow \begin{pmatrix} \rho_{00} & 0 \\ 0 & \rho_{11} \end{pmatrix}, \quad (1.140)$$

as the off-diagonal elements ρ_{01} and ρ_{10} —the *coherences* encoding the relative phase between $|0\rangle$ and $|1\rangle$ —are progressively suppressed by the coupling to the environment, while the populations remain unchanged. As a result, the system evolves

towards a mixed state, reflecting the loss of phase information due to correlations with the environment.

A good qubit is a quantum system capable of storing coherent quantum information for as long as possible. Moreover, it must allow for the creation, manipulation, and measurement of a quantum state before coherence is lost. This means that T_1 and T_2 must be much longer than the time required series of operations.

Trapped ion qubits are among the most coherent systems available, with coherence times reaching tens of seconds. Their gate operations are relatively slow, around $10\ \mu\text{s}$, but they can support millions of operations before decoherence. The main sources of error include motional heating of the ions and cross-talk between qubits due to shared phonon modes in the ion crystal. Laser intensity fluctuations and imperfect pulse shaping also contribute to gate infidelity [106].

Rydberg atom qubits offer faster gate operations and coherence times in the millisecond range. They rely on strong dipole-dipole interactions via excitation to Rydberg states. However, these excited states are prone to spontaneous decay and leakage outside the computational subspace. Additional errors arise from imperfect blockade mechanisms and laser phase noise, which can lead to errors during multi-qubit operations [107].

Superconducting qubits are known for their fast gate speeds, but they suffer from shorter coherence times. Charge qubits are highly sensitive to charge noise, which limits their practical use. Flux qubits are affected by magnetic flux noise and instability in the external control fields. Transmon qubits, which are designed to suppress charge noise, offer a good balance between coherence and speed [105].

Qubit Type	Coherence Time	Gate Time	Operational depth
Trapped ions	$\sim 10 - 100\ \text{s}$	$\sim 10\ \mu\text{s}$	$> 10^7$
Rydberg atoms	$\sim 1 - 10\ \text{ms}$	$100\ \text{ns} - 1\ \mu\text{s}$	$10^3 - 10^4$
Charge qubit	$\sim 1 - 10\ \mu\text{s}$	$1 - 10\ \text{ns}$	$10^2 - 10^3$
Flux qubit	$\sim 10 - 100\ \mu\text{s}$	$\sim 10\ \text{ns}$	$10^3 - 10^4$
Transmon qubit	$\sim 20 - 100\ \mu\text{s}$	$10 - 40\ \text{ns}$	$2 \times 10^3 - 10^4$

Table 1.1: Comparison of typical coherence times, gate durations, and operational depth for various qubit technologies.

In Table 1.1 is reported a summary of coherence times, gate durations, and operational depth, namely the number of operations that can be done within the coherence time, for the various qubit technologies presented in the Chapter.

It is worth noting that, as will be clear in the following, in the context of QBs, relaxation poses a fundamental challenge to the proper functioning of the devices.

Although trapped ion qubits exhibit very long coherence times and large operational depths, their practical scalability to large numbers of qubits is challenging. In contrast, superconducting transmon qubits, while having shorter coherence times, can be more easily scaled to multi-qubit architectures. This trade-off between coherence and scalability is a key factor in the choice of qubit technology for large-scale quantum computers.

Chapter 2

Quantum Batteries

Over the past decade, many models of QBs have been proposed, featuring various combinations of classical and quantum systems playing the roles of QB and charger. Since some of these models will be presented throughout this Thesis, the purpose of this Chapter is to introduce the formalism used to study QBs, describing the main figures of merit and two representative models of charging, one via classical drive [26] and the other via a quantum system [61]. The platforms described in the previous Chapter can be used to implement these systems in the laboratory. In recent years, experimental progress has been made. The first reported example of a QB, dating back to 2022, is based on fluorescent organic molecules placed inside a cavity [14]. In the more recent years, research has continued in this direction [37, 41, 108]. QBs have also been realized using superconducting circuits [24, 45], quantum dots [46] and solid-state implementations [43, 109].

2.1 General Model

In the following, the coupled QB and charger will be described by an Hamiltonian of the form

$$\hat{\mathcal{H}}_{sys}(t) = \hat{\mathcal{H}}_B + \hat{\mathcal{H}}_C + \hat{\mathcal{H}}_{int}(t) \quad (2.1)$$

with $\hat{\mathcal{H}}_B$ the QB's Hamiltonian, $\hat{\mathcal{H}}_C$ the charger's Hamiltonian and $\hat{\mathcal{H}}_{int}$ the interaction Hamiltonian between QB and charger. The latter is in general time-dependent, and in the QBs framework, one usually considers the situation in which

$$\hat{\mathcal{H}}_{int}(\bar{t}) = \hat{\mathcal{H}}_{int}(0) = 0. \quad (2.2)$$

This means that the interaction between the charger and the QB is switched on only for a given amount of time $\bar{t}$. In Fig. 2.1 is represented the scheme of a generic charging process. It is worth to note that Eq. (2.1) is written in a simplified notation. Being h_B and h_C respectively the Hilbert spaces of the QB and the charger, the interaction Hamiltonian $\hat{\mathcal{H}}_{int}$ must be applied to states in the Hilbert space $h_{sys} = h_B \otimes h_C$. The system Hamiltonian must more properly be written in h_{sys} as

$$\hat{\mathcal{H}}_{sys}(t) = \mathbb{I}_C \otimes \hat{\mathcal{H}}_B + \hat{\mathcal{H}}_C \otimes \mathbb{I}_B + \hat{\mathcal{H}}_{int}(t). \quad (2.3)$$

For sake of simplicity, however, in the following will be used the notation reported in Eq. (2.1).

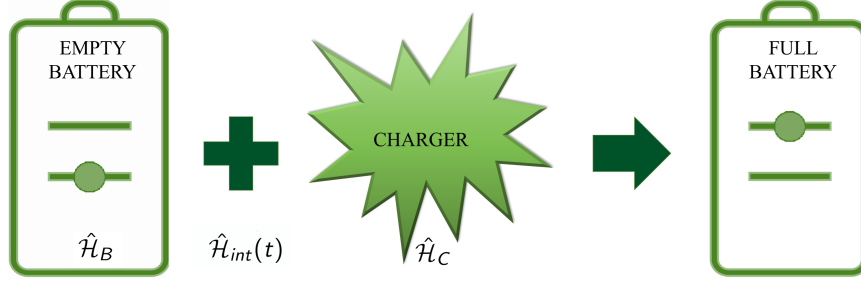


Figure 2.1: An empty QB ($\hat{\mathcal{H}}_B$), schematically represented as a TLS in its ground state, is coupled to a charger ($\hat{\mathcal{H}}_C$) via the interaction $\hat{\mathcal{H}}_{int}(t)$. Disconnecting the charger leaves the QB charged.

2.2 Figures of merit

The main figures of merit that we will use to characterize the performance of a QB are the stored energy, the average power, the time required to reach the maximum of these functions, and the ergotropy, namely the maximum work extractable from a system through unitary operations. Depending on the context, a central role may also be played by the work required to switch the interaction Hamiltonian on and off. Taking this into account, along with the previously mentioned quantities, different definitions of QB efficiency may be provided.

2.2.1 Stored Energy

One of the main figures of merit considered in the context of QB is the energy stored in a specific part of the system, usually the QB or the charger. It can be defined in two ways, depending on the model being considered. The first possibility is to define the energy stored in the system at a given time t ; in formula

$$E_i(t) = \langle \hat{\mathcal{H}}_i(t) \rangle \quad (2.4)$$

with $\langle \dots \rangle$ as defined in Eq. (1.23). The second possibility is to define the change in energy with respect to the initial value [10, 11]. In formula, it can be expressed as

$$\Delta E_i(t) = \langle \hat{\mathcal{H}}_i(t) \rangle - \langle \hat{\mathcal{H}}_i(0) \rangle. \quad (2.5)$$

In both definitions, $i = B, C$.

Maxima and minima of the energy stored

To analyze the charging and discharging processes of a QB, it is essential to identify the maxima and minima of the energy stored in the QB. The goal is to reach the maximum during the charging phase and the minimum during the discharging phase. We can therefore define

$$E_i^{max} = \max_t [E_i(t)] = E_i(t_{max}^{(E_i)}) \quad (2.6)$$

$$E_i^{min} = \min_t [E_i(t)] = E_i(t_{min}^{(E_i)}) \quad (2.7)$$

with $t_{max}^{(E_i)}$ and $t_{min}^{(E_i)}$ respectively the times at which the maximum and minimum of $E_i(t)$ are reached. In the case where $i = B$, they represent the charging and discharging times of the QB. If the values of $E_B^{max/min}$ are reached multiple times during the time evolution, the earliest times are conventionally considered, since it is generally preferable to charge/discharge the QB in the shortest possible time. In order to keep the notation easy to read, and because these quantities are usually referred to the QB, the subscript B will often be omitted and $E_B^{max/min}$ will be indicated only as $E_{max/min}$, for notational convenience.

A completely analogous reasoning can be made for $\Delta E_i(t)$, since the two quantities differ only by a constant. In this second case we would define ΔE_i^{max} , ΔE_i^{min} , $t_{max}^{(\Delta E_i)}$ and $t_{min}^{(\Delta E_i)}$.

Capacity

It is also possible to define how much energy can be stored in the QB. This quantity is also known as capacity and can be defined as

$$\mathcal{C}_B^{(E)} = \langle \uparrow | \hat{\mathcal{H}}_B | \uparrow \rangle - \langle \downarrow | \hat{\mathcal{H}}_B | \downarrow \rangle \quad (2.8)$$

where $|\downarrow\rangle$ and $|\uparrow\rangle$ are the empty and full state of the QB, respectively.

Note that more refined definitions for the capacity of a QB are possible indeed. The definition of capacity adopted in this work corresponds to the maximum theoretical amount of energy that could be stored in the QB. However, this definition does not guarantee that a unitary operation exists that actually brings the system from the empty state to the fully charged state. For a more complete discussion about this point see Ref. [110].

The quantity defined in Eq. (2.8) can, for example, be used as reference scale to plot energy. In this case we refer to the normalized stored energy as

$$\frac{\Delta E_B(t)}{\mathcal{C}_B^{(E)}}. \quad (2.9)$$

This choice will be done in Chapter 5.

2.2.2 Average Power

The second quantity considered is the average charging power. Although this can also be defined for all parts of the system, particularly for both the charger and the QB, generally only the power generated by the latter is taken into account. It can be defined as

$$P(t) = \frac{\Delta E_B(t)}{t}, \quad (2.10)$$

using the definition of energy in Eq. (2.5). It quantifies how much the energy stored in the QB varies over the time interval $[0, t]$. As in the case of energy, it is important to define the time at which the maximum power is reached, $t_{max}^{(P)}$

$$P^{max} = \max_t [P(t)] = P(t_{max}^{(P)}), \quad (2.11)$$

in general, $t_{max}^{(E_B)} \neq t_{max}^{(P)}$.

2.2.3 Ergotropy

The next figure of merit that we introduce is the ergotropy, namely the maximum work extractable with unitary operation from a system, in this context from the QB [60, 111]. In QBs one typically restricts to unitary operations because they enable work extraction through coherent, entropy-preserving transformations, ensuring that no energy is lost to dissipation and that quantum coherence, essential for quantum advantage, is maintained. In general, as defined in the previous Section, the energy stored in the QB is a function of time t . However, in order to define the ergotropy, it is more convenient to make it explicit that the energy stored in the QB is a function of the state of the system, and that this latter is function of time, namely

$$E_B(t) \equiv E_B(\rho(t)). \quad (2.12)$$

For notational convenience, in this Section it will be indicated as $E_B(\rho)$. It can be decomposed as

$$E_B(\rho) = \mathcal{E}(\rho) + E(\pi_\rho) \quad (2.13)$$

where $\mathcal{E}(\rho)$ is the ergotropy of ρ and $E(\pi_\rho) = \text{Tr}[\hat{\mathcal{H}}\pi_\rho]$ is the energy not extractable through unitary operations. The latter is associated to the *passive* state π_ρ of ρ , which is unitarily related to ρ via

$$\pi_\rho = \hat{U}\rho\hat{U}^\dagger, \quad (2.14)$$

The ergotropy is non-negative, $\mathcal{E}(\rho) \geq 0$, and zero if and only if ρ is passive, $\mathcal{E}(\pi_\rho) = 0$. Therefore, states with vanishing ergotropy, $\mathcal{E} = 0$, are referred to as *passive states* [112, 113], and those with finite ergotropy, $\mathcal{E} > 0$, as *active states*.

Given the diagonal representation of the density matrix

$$\rho(t) = \sum_n r_n(t) |r_n(t)\rangle\langle r_n(t)| \quad (2.15)$$

with $r_0(t) \geq r_1(t) \geq \dots$, we can associate to $\rho(t)$ a passive state $\pi_\rho(t)$, defined as the state that minimizes the average energy over all states unitarily connected to $\rho(t)$. This minimization is performed with respect to the system Hamiltonian $\hat{\mathcal{H}}$, whose eigenstates $|\epsilon_n\rangle$ are ordered such that $\epsilon_0 \leq \epsilon_1 \leq \dots$. Since unitary transformations preserve the spectrum of $\rho(t)$, the minimization of energy reduces to finding the unitary that assigns the largest eigenvalue $r_0(t)$ to the lowest energy eigenstate $|\epsilon_0\rangle$, the second largest $r_1(t)$ to $|\epsilon_1\rangle$, and so on. This assignment ensures that the resulting state has the lowest possible expectation value of energy among all unitarily equivalent states. The passive state is therefore diagonal in the energy eigenbasis and reads

$$\pi_\rho(t) = \sum_n r_n(t) |\epsilon_n\rangle\langle\epsilon_n|, \quad (2.16)$$

where the eigenvalues $r_n(t)$ of $\rho(t)$ are arranged in decreasing order and matched to the energy eigenstates in increasing order. This construction guarantees that no work can be extracted from $\pi_\rho(t)$ via unitary operations, as any such transformation would increase the system's energy. Among all unitaries connecting $\rho(t)$ to its passive counterpart, one can explicitly write a representative transformation as

$$\hat{U}(\boldsymbol{\theta}) = \sum_{n=0} e^{i\theta_n} |\epsilon_n\rangle\langle r_n|. \quad (2.17)$$

The phases $\boldsymbol{\theta} = \{\theta_n\}$ reflect the arbitrariness in the normalization of the eigenstates, and only $d - 1$ of them are physically relevant, as a global phase has no observable effect [114, 115]. These phases are typically neglected, as they do not affect either the passive state in Eq. (2.16) or the ergotropy.

This leads to the general definition

$$\mathcal{E}(\rho(t), \hat{\mathcal{H}}) = \sum_{k,n} r_k(t) \epsilon_n (|\langle r_k(t) | \epsilon_n \rangle|^2 - \delta_{k,n}). \quad (2.18)$$

In general setups, evaluating the ergotropy can be very challenging and often requires numerical methods. However, in certain cases, it is possible to make some simplification or even derive a closed-form expression. In the following Paragraphs, we will focus on some special cases that will be used in this Thesis.

Local VS Global ergotropy

The first aspect that it is worth to mention is that ergotropy is not an additive quantity. If we consider a composite system with a Hamiltonian given by a sum over k distinct terms, $\hat{\mathcal{H}} = \sum_k \hat{\mathcal{H}}_k$, its ergotropy is generally not equal to the sum of the ergotropies of its subsystems. This reflects the fact that the ergotropy depends on the structure of the quantum state, including coherences and correlations that may be inaccessible when subsystems are treated independently.

In multipartite systems, this distinction becomes evident when comparing work extraction under local versus global unitary operations. Local ergotropy refers to the work extractable by acting separately on each subsystem

$$\mathcal{E}^{(l)} = \sum_{k=1}^n \mathcal{E}_l^k(\rho_k), \quad (2.19)$$

where ρ_k is the reduced state of the k -th subsystem. In contrast, global ergotropy considers the full state ρ and the total Hamiltonian $\hat{\mathcal{H}}$, allowing for collective operations, as defined in the previous Section. Since π_ρ , defined in Eq. (2.14), is not generally equal to $\bigotimes_k \pi_{\rho_k}$, the two quantities differ, and global operations may unlock additional extractable work. This is a consequence of the fact that local unitary operations acting on a single subsystem are not enough in order to extract all the energy stored into the QB, and non-local unitary operations collectively acting on the whole QB are needed in order to extract also the energy trapped in the correlations among the elementary building blocks composing the device [7, 60]. There is, however, an exception. Indeed, when the passive state π_ρ of ρ is thermal, we have an extensive ergotropy $\mathcal{E}(\bigotimes_k \pi_{\rho_k}) = n\mathcal{E}(\rho)$ [116].

Ergotropy extraction from a qubit

In this Paragraph, we discuss the extraction of ergotropy from one qubit described by a real density matrix, as it is the building block of many models, including the one described in Chapter 3. As we have seen in Section 1.1, a qubit state ρ can be represented in the Bloch sphere as a point of coordinates (r_x, r_y, r_z) , where $r_i = \text{Tr}[\hat{\sigma}_i \rho]$ with $i = x, y, z$, and $r = \sqrt{r_x^2 + r_y^2 + r_z^2}$. In addition, if the density matrix is real, we have $r_y = 0$. The Hamiltonian of the system is $\hat{\mathcal{H}} = \Omega_z \hat{\sigma}_z$, with Ω_z the level spacing. In the unitary operation in Eq. (2.17) we said that there are only

$d - 1$ physical phases, and hence for a TLS, there is only one independent phase. The unitary can therefore be rewritten as

$$\hat{U}(\theta) = e^{-i\theta}|\epsilon_1\rangle\langle\lambda_1| + e^{i\theta}|\epsilon_2\rangle\langle\lambda_2|, \quad (2.20)$$

with $0 \leq \theta < \pi$. Recalling the convention on the sorting of the eigenvalues, the eigensystem of $\hat{\mathcal{H}}$ is

$$|\epsilon_1\rangle = |1\rangle, \quad |\epsilon_2\rangle = |0\rangle, \quad (2.21)$$

with $\epsilon_{1/2} = \mp\Omega_z$ and that of ρ is

$$|\lambda_1\rangle = |\lambda_+\rangle, \quad |\lambda_2\rangle = |\lambda_-\rangle \quad (2.22)$$

with $\lambda_{1/2} = \frac{1}{2}(1 \pm r)$ and $0 \leq r \leq 1$, as defined in Eq. (1.8).

Now we focus on the eigensystem of ρ . If ρ is a 2×2 real symmetric matrix, its eigenvectors can be expressed in the form $\alpha|0\rangle + \beta|1\rangle$ and $-\beta|0\rangle + \alpha|1\rangle$, with $\alpha, \beta \in \mathbb{R}$. Accordingly, we can rewrite the eigenstates in Eq. (1.8) as

$$\begin{aligned} |\lambda_2\rangle \equiv |\lambda_-\rangle &= \cos\alpha|0\rangle + \sin\alpha|1\rangle, \\ |\lambda_1\rangle \equiv |\lambda_+\rangle &= -\sin\alpha|0\rangle + \cos\alpha|1\rangle, \end{aligned} \quad (2.23)$$

with

$$\cos\alpha = -\frac{r_x}{\sqrt{2r(r+r_z)}}, \quad \sin\alpha = \frac{r+r_z}{\sqrt{2r(r+r_z)}}, \quad (2.24)$$

where $r = \sqrt{r_x^2 + r_z^2}$ (recall that $r_y = 0$, being ρ real), from which $\tan\alpha = -(r+r_z)/r_x$. Note that $r+r_z \geq 0$ always. Then, we can write the unitary operator in Eq. (2.20) as

$$\begin{aligned} \hat{U}(\theta) &= e^{i\theta} \cos\alpha|0\rangle\langle 0| + e^{i\theta} \sin\alpha|0\rangle\langle 1| \\ &\quad - e^{-i\theta} \sin\alpha|1\rangle\langle 0| + e^{-i\theta} \cos\alpha|1\rangle\langle 1|. \end{aligned} \quad (2.25)$$

It is possible to rewrite it in terms of

$$e^{i\theta\hat{\sigma}_z} = \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix}, \quad e^{i\alpha\hat{\sigma}_y} = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}. \quad (2.26)$$

Since any unitary operation on a qubit corresponds to a rotation of the Bloch vector that preserves its norm, it can always be represented as a composition of rotations around two axes. In particular, the decomposition $e^{i\theta\hat{\sigma}_z}e^{i\alpha\hat{\sigma}_y}$ shows explicitly that any such unitary maps one point on the Bloch sphere to another through a rotation by an angle α around the y axis followed by a rotation by an angle θ around the z axis. Thus, the pair of angles (θ, α) fully characterizes the unitary.

In conclusion, to extract ergotropy from a qubit, we have to apply the unitary operation [114]

$$\hat{U}(\theta) = \begin{pmatrix} e^{i\theta} \cos\alpha & e^{i\theta} \sin\alpha \\ -e^{-i\theta} \sin\alpha & e^{-i\theta} \cos\alpha \end{pmatrix} = e^{i\theta\hat{\sigma}_z}e^{i\alpha\hat{\sigma}_y}, \quad (2.27)$$

where $0 \leq \theta < \pi$ is an independent arbitrary phase and $\alpha = \arctan[-(r+r_z)/r_x]$.

Thermal state

The concept of passivity, already introduced, was first formalized by Pusz and Woronowicz in 1978 [112]. In their seminal work, they proved that only thermal states and ground states are *completely passive*, meaning that no work can be extracted from any number of copies via unitary operations.

Passive states (see Eq. (2.14)) are defined as those that commute with the system Hamiltonian and exhibit no population inversion [60, 112, 113]. A prominent subclass of passive states is given by thermal (or Gibbs) states, which take the form

$$\tau_\beta = \frac{e^{-\beta\hat{\mathcal{H}}}}{\text{Tr}[e^{-\beta\hat{\mathcal{H}}}]}$$
(2.28)

with $\beta = T^{-1}$ (from now on we will assume $k_B = 1$). Using the definitions above, it can be explicitly written as

$$\tau_\beta = \sum_{k=1}^d \frac{e^{-\beta\epsilon_k}}{\text{Tr}[e^{-\beta\hat{\mathcal{H}}}] } |\epsilon_k\rangle\langle\epsilon_k|.$$
(2.29)

While passive states do not allow for work extraction from a single copy, work can be extracted from multiple copies via collective unitary operations, except in the case of thermal states [7, 116]. For this reason, thermal states (including the ground state at $T = 0$) are referred to as completely passive: a state ρ is completely passive if $\bigotimes_n \rho$ remains passive for all $n = 1, 2, \dots$, with respect to the additive Hamiltonian

$$\hat{\mathcal{H}}^{(n)} = \sum_{k=1}^n \hat{\mathcal{H}}_k,$$
(2.30)

where each $\hat{\mathcal{H}}_k$ is an independent copy of $\hat{\mathcal{H}}$ [112, 113].

In the case of a TLS, the notions of passivity and thermality coincide. Consider a Hamiltonian

$$\hat{\mathcal{H}} = \varepsilon_0|0\rangle\langle 0| + \varepsilon_1|1\rangle\langle 1|$$
(2.31)

with $\varepsilon_1 > \varepsilon_0$. Any state diagonal in the energy basis can be written as

$$\rho = p_0|0\rangle\langle 0| + p_1|1\rangle\langle 1|, \quad p_0 + p_1 = 1.$$
(2.32)

The state is passive if and only if $p_0 \geq p_1$, meaning the ground state is more populated than the excited state. This condition uniquely determines a Boltzmann distribution for some $\beta > 0$, implying that ρ must be thermal. Thus, every passive state in a TLS is necessarily a thermal state.

However, this equivalence breaks down in systems with three or more energy levels. In such cases, one can construct passive states whose populations decrease with energy but do not follow a Boltzmann distribution. These states are passive—since no unitary can lower their energy—but they cannot be written as τ_β for any β . This illustrates that passivity is a broader concept than thermality in higher-dimensional quantum systems. These observations will be relevant in Chapter 3.

Gaussian states

Speaking about ergotropy, a class of states that is particular worth to mention is the one of the Gaussian states of an harmonic oscillator, with Hamiltonian

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + \frac{m\omega_0^2}{2}\hat{x}^2 \quad (2.33)$$

where $\hat{x}$ and $\hat{p}$ are respectively the position and its conjugate momentum, m and ω_0 its mass and its characteristic frequency respectively. In this case, it is possible to derive a closed expression to evaluate the ergotropy [117, 118]. If the state of the QB remains Gaussian at any time t (see Ref. [36] for more details), its ergotropy is given by

$$\mathcal{E}(t) = \langle \hat{\mathcal{H}}_B(t) \rangle - \omega_0 \sqrt{\det \sigma_B(t)}, \quad (2.34)$$

where $\sigma_B(t)$ is the covariance matrix [119] at time t ,

$$\sigma_B(t) = m \begin{pmatrix} \omega_0 \langle \hat{x}^2(t) \rangle & \frac{1}{2} \frac{d}{dt} \langle \hat{x}^2(t) \rangle \\ \frac{1}{2} \frac{d}{dt} \langle \hat{x}^2(t) \rangle & \frac{1}{\omega_0} \langle \hat{x}^2(t) \rangle \end{pmatrix} \quad (2.35)$$

with $\hat{x} = \hat{p}/m$. This formula will be crucial in Chapter 4.

2.2.4 Work Cost of Interaction Switching

Before concluding this Section, and to be able to give a proper thermodynamic characterization of QB, it is important to introduce the work needed to switch on and off the interaction Hamiltonian [59]. As introduced in Eq. (2.2), $\hat{H}_{int}(t)$ is usually switch on and off at time $t = 0$ and $t = \bar{t}$, respectively. The cost associated with these operations is

$$W(t) = W_{\text{on}} + W_{\text{off}}(t), \quad (2.36)$$

where

$$W_{\text{on}} = \langle \hat{H}_{int}(0) \rangle \quad W_{\text{off}}(\bar{t}) = -\langle \hat{H}_{int}(\bar{t}) \rangle. \quad (2.37)$$

These expressions are valid under the assumption of very short switching on and off times of the coupling between the QB and the charger. In the case of a much smoother switching, modeled by means of a more general function $\lambda(t)$, the quantities W_{on} and W_{off} would be given by the integral the power associated with the external driving

$$W_{\text{sw}} = \int_{t_i}^{t_f} \dot{\lambda}(t) \langle \hat{\mathcal{H}}_{\text{int}}(t) \rangle dt, \quad (2.38)$$

where $\hat{\mathcal{H}}_{\text{int}}(t)$ is the interaction Hamiltonian [15]. In the following, however, we shall assume the limit of an instantaneous (fast) switch on/off, which allows us to treat the coupling as a step function and simplify the energy exchange analysis.

In analogy with what defined in Eq. (2.5), the total work can be alternatively written as

$$W(t) = - \left[\langle \hat{H}_{int}(t) \rangle - \langle \hat{H}_{int}(0) \rangle \right] = -\Delta E_{int}(t). \quad (2.39)$$

If the total system is closed, after the switching on, we can write the total energy balance

$$\Delta E_B(t) + \Delta E_C(t) = W(t) \quad (2.40)$$

with a clear meaning: the total work $W(t)$ is distributed among the accumulated energy of the battery $\Delta E_B(t)$ and the energy exchanged with the charger at time t .

To better clarify the quantities defined in this Section, it is useful to analyze the charging of a QB in the case of two exemplary models characterized by a classical and a quantum charger.

2.3 Few levels QBs charged by a classical charger

The first examples of QB that we present are two- and three-level QBs charged by a time-dependent classical charger [25, 26]. In literature, there are many examples of models based on classical chargers [16, 23, 120], including an experimental evidence of a three-level QB realized with a superconducting circuit in the transmon regime [24]. In this Section we will show that a full analytical description of these systems dynamics is possible under very general conditions. We will identify fast stable protocols able to realize an almost complete charging of the QB and we will describe the simulation of these protocols on IBM quantum devices based on superconducting circuits in the transmon regime (see Section 1.2.3). The results of this work have been published in Ref. [26] and the present Section is largely based upon it.

2.3.1 Two level QB

Let's start by considering a QB described by a TLS with Hamiltonian

$$\hat{\mathcal{H}}_B^{(2)} = \omega_0 |0\rangle\langle 0| + \omega_1 |1\rangle\langle 1| \quad (2.41)$$

with level spacing

$$\Delta = \omega_1 - \omega_0 \quad (2.42)$$

between the ground state $|0\rangle$ and the first excited state $|1\rangle$ (from now on we assume $\hbar = 1$). The dynamics of the QB is controlled by a classical external time-dependent drive. The total Hamiltonian reads [47, 121]

$$\hat{\mathcal{H}}^{(2)}(t) = \hat{\mathcal{H}}_B^{(2)} + \hat{\mathcal{H}}_{int}^{(2)}(t) \quad (2.43)$$

here

$$\hat{\mathcal{H}}_{int}^{(2)}(t) = gf(t) \cos(\Omega_1 t) (|0\rangle\langle 1| + |1\rangle\langle 0|). \quad (2.44)$$

with $f(t)$ is a time-dependent envelop function with maximum amplitude equal to 1, whose form will be specified in the following. Such function is further modulated by a cosine with controllable frequency Ω_1 . Finally, g represents the intensity of the (dipole) coupling between the QB and the classical drive. Notice that in this model we can neglect the dynamics of the charger ($\hat{\mathcal{H}}_C$ in Eq. (2.1)) because, being a classical object, it is not affected by the state of the QB [120].

We can now consider the generic initial wave-function at time $t = 0$ [25]

$$|\psi(0)\rangle = \sqrt{a} |0\rangle + \sqrt{1-a} e^{i\phi} |1\rangle, \quad (2.45)$$

with $0 \leq a \leq 1$ and $0 \leq \phi < 2\pi$ real parameters. The experimentally realized transmon devices, including the devices developed by IBM, usually satisfy $g \ll \Delta$ [105].

Under this condition, in order to achieve a complete charging of the QB, namely a perfect transition $|0\rangle \rightarrow |1\rangle$, it is necessary to set $\Omega_1 = \Delta$, the frequency of the drive must be in resonance with the level spacing of the qubit.

In order to analytically solve the problem, it is useful to consider the time-dependent rotation

$$\hat{S}^{(2)}(t) = e^{i\hat{\mathcal{H}}_B^{(2)}t} \quad (2.46)$$

leading, in the rotating frame, to the new Hamiltonian

$$\hat{\mathcal{H}}'^{(2)} = \hat{S}^{(2)}\hat{\mathcal{H}}^{(2)}(\hat{S}^{(2)})^\dagger - i\hat{S}^{(2)}\frac{d(\hat{S}^{(2)})^\dagger}{dt}. \quad (2.47)$$

Under the conditions of resonance and small coupling discussed above, we can safely consider the rotating wave approximation (RWA) [122–125]. Doing this, we obtain the effective Hamiltonian

$$\hat{\mathcal{H}}_{eff}^{(2)}(t) = \frac{g}{2}f(t)(|0\rangle\langle 1| + |1\rangle\langle 0|), \quad (2.48)$$

neglecting a constant term that plays no role in the dynamics. This leads to the Schrödinger equation, introduced in Section 1.1.2

$$i\left|\dot{\psi}'(t)\right\rangle = \hat{\mathcal{H}}_{eff}^{(2)}|\psi'(t)\rangle \quad (2.49)$$

where $|\psi'(t)\rangle = \hat{S}^{(2)}(t)|\psi(t)\rangle$ with $|\psi(t)\rangle$ the wave-function of the qubit at a given time [25].

We can now evaluate the energy stored in the QB defined in Eq. (2.4). According to this definition and taking into account the analysis reported above, the energy stored into the QB at the time t can be explicitly written (assuming for now on ω_0 as the energy reference) as

$$E_B^{(2)}(t) = \Delta \left[a \sin^2 \frac{\theta(t)}{2} + (1-a) \cos^2 \frac{\theta(t)}{2} \right] \quad (2.50)$$

$$+ 2\sqrt{a}\sqrt{1-a} \sin \phi \sin \frac{\theta(t)}{2} \cos \frac{\theta(t)}{2}, \quad (2.51)$$

where

$$\theta(t) = g \int_0^t f(t') dt'. \quad (2.52)$$

According to this expression, the parameter that control the system's dynamics is the area under the envelope function $f(t)$. However, in order to explicitly evaluate the energy stored into the QB as a function of time it is necessary to specify the form of $f(t)$. A good choice for the envelope function is

$$f(t) = \mathcal{N} e^{-\frac{(t-t_m/2)^2}{2\sigma^2}}, \quad (2.53)$$

a Gaussian with amplitude $\mathcal{N}$ and standard deviation σ , centered at $t = t_m/2$, with t_m the time at which the measurement of the state is carried out [25]. In the following we will assume

$$\sigma = \frac{t_m}{8}, \quad (2.54)$$

in order to have $t_m \gg \sigma$ and fulfill the condition in Eq. (2.2). Moreover we have

$$\mathcal{N} = \frac{\theta_m}{(g\sigma\sqrt{2\pi})}, \quad (2.55)$$

with θ_m the total phase induced by the application of the pulse.

Indeed, we have

$$\theta(t) \approx \frac{\theta_m}{2} \left[\text{Erf} \left(\frac{t - \frac{t_m}{2}}{\sqrt{2}\sigma} \right) + 1 \right], \quad (2.56)$$

with $\text{Erf}(x)$ the error function of argument x . This leads to $\theta \approx \theta_m$ for $t \approx t_m \gg \sigma$.

Replacing the above expression into Eq. (2.51) we can determine the charging time t_c , namely the time at which the QB is (almost) completely charged, as a fraction of t_m . For example, in Fig. 2.2, the QB reaches a charging $E_{thr}^{(2)} = 0.95\Delta$ in a time $t_c = 0.59t_m$.

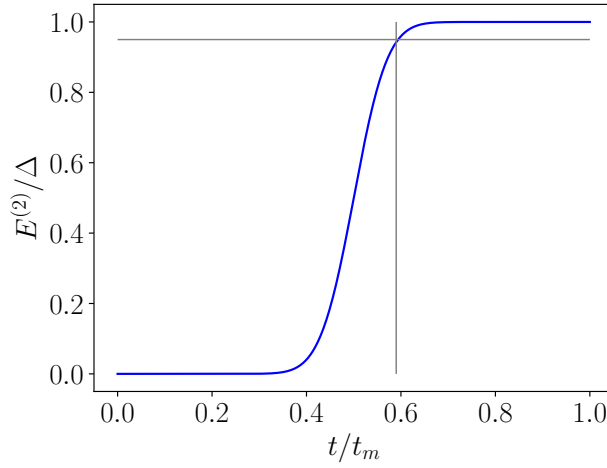


Figure 2.2: Blue curve: theoretical behavior of the energy $E^{(2)}$ stored into the qubit QB (in units of Δ) as a function of t (in units of t_m) and with initial condition $|\psi(t)\rangle = |0\rangle$ ($a = 1$ and arbitrary ϕ in Eq. (2.45)). Horizontal grey line indicates a QB charging of $E_{thr}^{(2)} = 0.95\Delta$, while the vertical grey line is in correspondence with the charging time $t_c = 0.59t_m$. Here we are considering $\theta_m = \pi$. Image taken from [26].

Obviously, the arbitrary choice of the value for the threshold $E_{thr}^{(2)}$ could play in general a relevant role in determining the charging time. However, assuming $E_{thr}^{(2)}$ ranging from 0.92Δ to 0.99Δ the charging times are only marginally different, namely $t_c \approx 0.6t_m$ (see Table 2.1). This strengthens the validity of our estimation.

E_{thr}/Δ	t_c/t_m
0.92	0.58
0.95	0.59
0.99	0.63

Table 2.1: Charging times (in units of t_m) for different values of the energy threshold (in unit of Δ).

Simulation on IBM quantum computer

Taking into account the above analysis, we now want to move to the simulation of this charging protocol on IBM quantum computer [47, 49]. It is worth to note, however, that the charging behavior in real time cannot be directly addressed, since real-time continuous measurements are not accessible in standard circuit-based quantum hardware. The only possibility is to reconstruct it starting from the evolution of the stored energy by fixing the time at $t = t_m \gg \sigma$ and by changing the amplitude of the applied pulse θ_m . According to this we have

$$E^{(2)}(\theta_m) = a \sin^2 \frac{\theta_m}{2} + (1 - a) \cos^2 \frac{\theta_m}{2} + 2\sqrt{a}\sqrt{1-a} \sin \phi \sin \frac{\theta_m}{2} \cos \frac{\theta_m}{2}, \quad (2.57)$$

with $\theta_m \equiv \theta(t = t_m)$. In Fig. 2.3 the real data extracted from the IBM quantum machine `ibm_auckland`¹ are shown compared to the theoretical prediction in the case of an ideal charging starting from the ground state $|0\rangle$. Data are extracted from the machine following the calibration procedure described in App. A [25, 26, 105]. Taking into account the fact that for this specific experiment $t_m = 30$ ns and

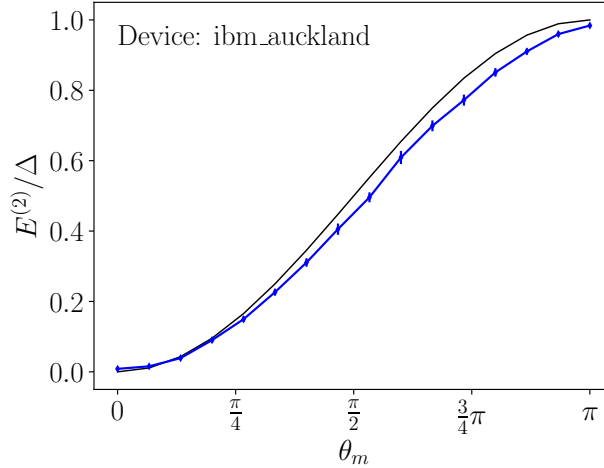


Figure 2.3: Energy stored in the QB (in units of Δ) as a function of θ_m . The black line is obtained analytically using Eq. (2.57) and with initial condition $|\psi(t)\rangle = |0\rangle$ ($a = 1$ and arbitrary ϕ in Eq. (2.45)). The blue points correspond to experimental data obtained from the `ibm_auckland` device, using the Gaussian pulses described in the main text with $t_m = 30$ ns. Image taken from [26].

due to the above considerations, one can estimate a charging time $t_c \approx 20$ ns.

2.3.2 Three level QB

We can now study the dynamics of a qutrit QB, addressing the ground ($|0\rangle$) and first two excited states ($|1\rangle, |2\rangle$) of a transmon (see Section 1.2.3). The QB is described by the Hamiltonian

$$\hat{\mathcal{H}}_B^{(3)} = \omega_0 |0\rangle\langle 0| + \omega_1 |1\rangle\langle 1| + \omega_2 |2\rangle\langle 2|. \quad (2.58)$$

¹Machine composed by 27 transmon circuits, of which we address the number 0 that is characterized by the the best compromise between the longer relaxation and dephasing times and the smaller read-out error. This device has been officially retired by IBM on November 9th, 2023.

As in the previous case, the dynamics is controlled by classical external drives such that

$$\hat{\mathcal{H}}^{(3)}(t) = \hat{\mathcal{H}}_B^{(3)} + \hat{\mathcal{H}}_{int}^{(3)}(t) \quad (2.59)$$

with

$$\hat{\mathcal{H}}_{int}^{(3)}(t) = g f_1(t) \cos(\Omega_1 t) (|0\rangle\langle 1| + |1\rangle\langle 0|) + g f_2(t) \cos(\Omega_2 t) (|1\rangle\langle 2| + |2\rangle\langle 1|). \quad (2.60)$$

Here, $f_1(t)$ and $f_2(t)$ are two generally different time-dependent envelope functions generalizing what shown in the previous Section.

It is worth to note that, despite the fact that a transition $|0\rangle \leftrightarrow |2\rangle$ could be useful for the following analysis, the general form of the classical driving Hamiltonian in Eq. (2.60) does not allow a direct transition between $|0\rangle$ and $|2\rangle$, but only between states with opposite parity ($|0\rangle \leftrightarrow |1\rangle$, $|1\rangle \leftrightarrow |2\rangle$). The Hamiltonian in Eq. (2.60) has been also investigated in Ref. [24] assuming an adiabatic evolution where the functions $f_1(t)$ and $f_2(t)$ were properly constrained at the level of the maximum admissible amplitude. However, in the following we will discuss more versatile and efficient charging protocols, leading to a faster and stable charging.

Proceeding in full analogy with what done in the case of the qubit QB we can consider a time-dependent rotation of the form

$$\hat{S}^{(3)}(t) = e^{i\hat{\mathcal{H}}_B^{(3)}t} \quad (2.61)$$

to describe the system in the rotating frame. In order to simplify the notation we can define

$$\Delta = \omega_1 - \omega_0, \quad (2.62)$$

$$\Delta' = \omega_2 - \omega_1. \quad (2.63)$$

Recalling Eq. (1.134) for the energy levels of a transmon we have that $\Delta > \Delta'$. It is worth to note that the condition $g \ll \Delta, \Delta'$ is typically well fulfilled.

Considering again the RWA, valid for $\Omega_1 = \Delta$ and $\Omega_2 = \Delta'$, the effective Hamiltonian in the rotating frame can be evaluate by means of the relation

$$\hat{\mathcal{H}}'^{(3)}(t) = \hat{S}^{(3)} \hat{\mathcal{H}}^{(3)} (\hat{S}^{(3)})^\dagger - i \hat{S}^{(3)} \frac{d(\hat{S}^{(3)})^\dagger}{dt} \quad (2.64)$$

and reads

$$\hat{\mathcal{H}}_{eff}^{(3)} = \frac{g}{2} f_1(t) (|0\rangle\langle 1| + |1\rangle\langle 0|) \quad (2.65)$$

$$+ \frac{g}{2} f_2(t) (|1\rangle\langle 2| + |2\rangle\langle 1|). \quad (2.66)$$

This leads to the Schrödinger equation

$$i \left| \dot{\Psi}'(t) \right\rangle = \hat{\mathcal{H}}_{eff}^{(3)} |\Psi'(t)\rangle \quad (2.67)$$

where $|\Psi'(t)\rangle = \hat{S}^{(3)}(t) |\Psi(t)\rangle$ with $|\Psi(t)\rangle$ the wave-function of the qutrit at a given time.

Considering the conventional spinorial notation

$$|\Psi'(t)\rangle = \begin{pmatrix} c_2(t) \\ c_1(t) \\ c_0(t) \end{pmatrix} \quad (2.68)$$

the dynamics of the system is described by this set of differential equations

$$\begin{pmatrix} \dot{c}_2(t) \\ \dot{c}_1(t) \\ \dot{c}_0(t) \end{pmatrix} = -i\frac{g}{2} \begin{pmatrix} 0 & f_2(t) & 0 \\ f_2(t) & 0 & f_1(t) \\ 0 & f_1(t) & 0 \end{pmatrix} \begin{pmatrix} c_2(t) \\ c_1(t) \\ c_0(t) \end{pmatrix}. \quad (2.69)$$

According to the previous discussion, in order to excite the QB from $|0\rangle$ to $|2\rangle$ we have to apply two pulses to the system. In order to achieve this goal in the two following Paragraphs of this Section we will describe two different options: the two pulses are applied sequentially and the two pulses are simultaneous. Both these cases can be treated analytically. From a theoretical point of view, also intermediate situations, where the two pulses partially overlap, can be studied by considering a numerical approach, however we are not going to discuss these cases because it is not easy to directly implement them on IBM machines [49]. It is worth to note that, beside the application in the framework of QBs, a deeper understanding of the dynamics of a qutrit is relevant to characterize the behavior of quantum devices outside the conventional schemes of quantum computation [126].

In the following, we will assume the ground state of the qutrit as initial state, namely

$$|\Psi(0)\rangle = |0\rangle. \quad (2.70)$$

Sequential charging protocol

The first charging protocol presented for the qutrit QB is the one where the two pulses are applied sequentially. We can choose two identical pulses, but properly delayed in time, namely $f_2(t) = f_1(t - t_m/2)$ and with $f_1(t)$ of the same Gaussian form as in Eq. (2.53) but with $t_m \rightarrow t_m/2$, in such a way that the total duration of the protocol is t_m . In this limit, the problem can be solved in two steps, each one identical to what previously discussed in the case of the qubit in Section 2.3.1. This is true because it is possible to assume that $f_1(t)$ is non zero only in the interval $t \in [0, t_m/2]$ and $f_2(t)$ in $t \in [t_m/2, t_m]$.

The first transition is so described by this set of differential equations

$$\begin{pmatrix} \dot{c}_2(t) \\ \dot{c}_1(t) \\ \dot{c}_0(t) \end{pmatrix} = -i\frac{g}{2} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & f_1(t) \\ 0 & f_1(t) & 0 \end{pmatrix} \begin{pmatrix} c_2(t) \\ c_1(t) \\ c_0(t) \end{pmatrix} \quad (2.71)$$

and the energy stored in the QB in this phase is (see Eq. (2.51) with $a = 1$)

$$E_{seq}^{(3)}(t) = \Delta \sin^2 \frac{\theta_1(t)}{2} \quad (2.72)$$

with

$$\theta_1(t) = g \int_0^t f_1(t') dt'. \quad (2.73)$$

For the second transition we need to solve the set of differential equations

$$\begin{pmatrix} \dot{c}_2(t) \\ \dot{c}_1(t) \\ \dot{c}_0(t) \end{pmatrix} = -i\frac{g}{2} \begin{pmatrix} 0 & f_2(t) & 0 \\ f_2(t) & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} c_2(t) \\ c_1(t) \\ c_0(t) \end{pmatrix}. \quad (2.74)$$

Assuming that in the first step the system reaches the first excited state ($|\Psi(t_m/2)\rangle \approx |1\rangle$), the energy stored in the QB is given by

$$E_{seq}^{(3)}(t) = \Delta + \Delta' \sin^2 \frac{\theta_2(t)}{2} \quad (2.75)$$

with

$$\theta_2(t) = g \int_{\frac{t_m}{2}}^t f_2(t') dt' \quad (2.76)$$

and $t \in [t_m/2, t_m]$.

Using the same Gaussian envelope function discussed in Section 2.3.1, with $\sigma = t_m/16$, we get

$$\theta_1(t) \approx \frac{\theta_{1,m}}{2} \left[\text{Erf} \left(\frac{t - \frac{t_m}{4}}{\sqrt{2}\sigma} \right) + 1 \right] \quad (2.77)$$

$$\theta_2(t) \approx \frac{\theta_{2,m}}{2} \left[\text{Erf} \left(\frac{t - \frac{3t_m}{4}}{\sqrt{2}\sigma} \right) + 1 \right]. \quad (2.78)$$

In Fig. 2.4 is shown the energy stored in the QB as a function of time. Here, one can clearly see a two-step charging (blue curve).

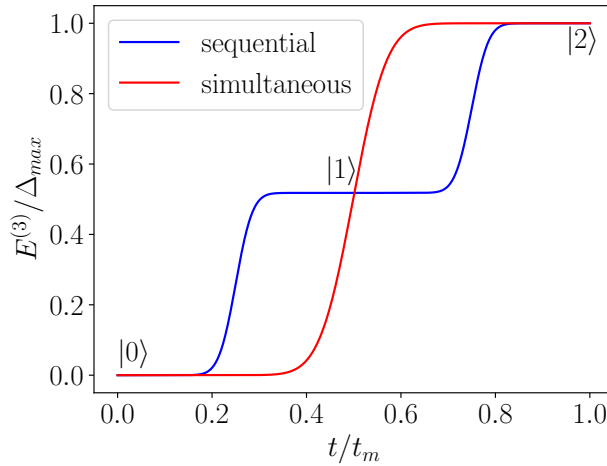


Figure 2.4: Energy stored in the QB (in units of $\Delta_{max} = \Delta + \Delta'$) as a function of t (in units of t_m) for both a sequential (blue curve) and simultaneous (red curve) charging protocol. Here we have considered pulses of Gaussian form satisfying the constraints discussed in the main text. Image taken from [26].

Simultaneous charging protocol

In this case the two pulses are applied at the same time, we can choose $f_1(t) = f_2(t) = f(t)$, which leads to the set of differential equation

$$\begin{pmatrix} \dot{c}_2(t) \\ \dot{c}_1(t) \\ \dot{c}_0(t) \end{pmatrix} = -i \frac{g}{2} f(t) \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} c_2(t) \\ c_1(t) \\ c_0(t) \end{pmatrix}. \quad (2.79)$$

The matrix

$$\hat{T} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad (2.80)$$

is diagonalized by means of the unitary transformation

$$\hat{U} = \begin{pmatrix} \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{pmatrix}. \quad (2.81)$$

This leads to new set of the decoupled equations

$$\begin{pmatrix} \dot{c}_-(t) \\ \dot{c}_+(t) \\ \dot{c}_B(t) \end{pmatrix} = -i\frac{g}{2}f(t) \begin{pmatrix} -\sqrt{2}c_-(t) \\ \sqrt{2}c_+(t) \\ 0 \end{pmatrix} \quad (2.82)$$

$$\rightarrow \begin{cases} c_-(t) = e^{i\frac{g}{\sqrt{2}}\int_0^t f(t')dt'} c_-(0) \\ c_+(t) = e^{-i\frac{g}{\sqrt{2}}\int_0^t f(t')dt'} c_+(0) \\ c_B(t) = c_B(0). \end{cases} \quad (2.83)$$

In this basis the state at time t is given by

$$|\Psi'(t)\rangle = \begin{pmatrix} e^{i\Theta(t)}c_-(0) \\ e^{-i\Theta(t)}c_+(0) \\ c_B(0) \end{pmatrix} \quad (2.84)$$

with

$$\Theta(t) = \frac{g}{\sqrt{2}} \int_0^t f(t')dt'. \quad (2.85)$$

Is this new basis the initial conditions lead to

$$\begin{pmatrix} c_-(0) \\ c_+(0) \\ c_B(0) \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \quad (2.86)$$

and consequently

$$|\Psi'(t)\rangle = \begin{pmatrix} \frac{1}{2}e^{i\Theta(t)} \\ \frac{1}{2}e^{-i\Theta(t)} \\ \frac{1}{\sqrt{2}} \end{pmatrix}. \quad (2.87)$$

Returning back to the original basis we finally have

$$|\Psi(t)\rangle = \begin{pmatrix} \frac{1}{2} [\cos \Theta(t) - 1] \\ -\frac{i}{\sqrt{2}} \sin \Theta(t) \\ \frac{1}{2} [\cos \Theta(t) + 1] \end{pmatrix}. \quad (2.88)$$

Considering the same Gaussian pulse as in the qubit case we obtain

$$\Theta(t) = \frac{\Theta_m}{2} \left[\text{Erf} \left(\frac{t - \frac{t_m}{2}}{\sqrt{2}\sigma} \right) + 1 \right] \quad (2.89)$$

with $\Theta_m = \theta_m/\sqrt{2}$.

In Fig. 2.4 we report the energy stored in the QB as a function of time (red curve), given by

$$E_{sim}^{(3)}(t) = \frac{\Delta}{2} \sin^2 \Theta(t) + \frac{\Delta_{max}}{4} [1 - \cos \Theta(t)]^2. \quad (2.90)$$

As expected, the complete charging of the QB can be obtained here in a unique step as long as $\Theta_m = \pi$.

Simulation on IBM quantum computer

As in the qubit case, we now want to show how it is possible to simulate these charging protocols in an IBM quantum computer. As before, the real time dynamics cannot be accessed directly, it is however possible to proceed in analogy with what done for the qubit, extracting it from the behavior of the energy stored at the final measurement time $t = t_m$ and changing the pulse amplitude. In order to do so we need to define for each protocol a quantity analogous to θ_m . For the sequential protocol it is convenient to define

$$\varphi_m = \begin{cases} \theta_{1,m} & \text{if } \theta_{1,m} \in [0, \pi] \\ \pi + \theta_{2,m} & \text{if } \theta_{1,m} = \pi \text{ \& } \theta_{2,m} \in [0, \pi]. \end{cases} \quad (2.91)$$

This definition lead to keep track of the fact that as long as the total amplitude is smaller then π we are considering the $|0\rangle \rightarrow |1\rangle$, while for a total amplitude greater than π we are addressing the $|1\rangle \rightarrow |2\rangle$ transition. In contrast, for the simultaneous protocol we can directly use Θ_m .

In terms of these variables we can explicit the energy stored in the QB in the sequential protocol

$$E_{seq}^{(3)}(\varphi_m) = \begin{cases} \frac{\Delta}{2} \sin^2 \frac{\varphi_m}{2} & \text{if } \varphi_m \in [0, \pi] \\ \Delta + \Delta' \sin^2 \left(\frac{\varphi_m - \pi}{2} \right) & \text{if } \varphi_m \in [\pi, 2\pi] \end{cases} \quad (2.92)$$

and in the simultaneous one

$$E_{sim}^{(3)}(\Theta_m) = \frac{\Delta}{2} \sin^2 \Theta_m + \frac{\Delta_{max}}{4} [1 - \cos \Theta_m]^2. \quad (2.93)$$

The behavior of the above functions, together with the relative experimental data obtained using respectively the `ibm_auckland` and `ibmq_toronto`² devices are reported in Fig. 2.5. Data are extracted from the machine following the calibration procedure described in App. A.

For the sequential charging protocol the agreement between data and the theoretical function is very good, in particular in the first half of each step. However, the experimental data show that it is not possible to fully charge the QB. Indeed, the maximum energy reached is 92.1% of the maximum energy $\Delta_{max} = \Delta + \Delta'$ ($\Delta_{max} = 39.2 \mu\text{eV}$). Here, the charging occurs in a time $t_c \approx 25$ ns. For what is concerning the simultaneous charging protocol, the maximum energy reached is 92.0% of Δ_{max} . This indicates that efficiencies of the two considered protocols are very

²Machine composed by 27 transmon circuits, of which we address the number 16 that is characterized by the best compromise between the longer relaxation and dephasing times and the smaller read-out error. This device has been officially retired by IBM on April 10th, 2023.

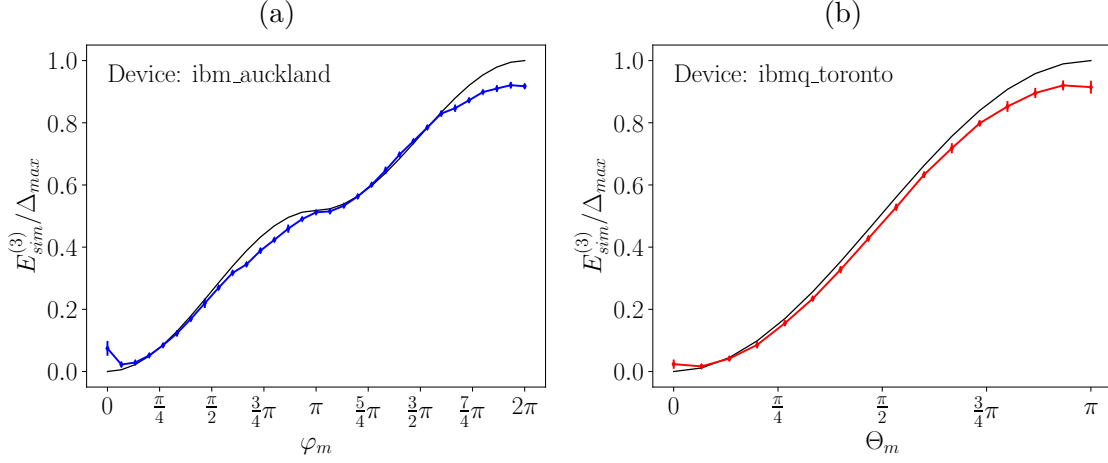


Figure 2.5: (a) Energy stored in the QB (in units of Δ_{max}) as a function of φ_m following the sequential charging protocol. The black line is obtained analytically using Eq. (2.92). The blue points correspond to experimental data obtained from the *ibm_auckland* device, using the Gaussian pulses described in the main text with $t_m = 30$ ns. (b) Energy stored in the QB (in units of Δ_{max}) as a function of Θ_m following the simultaneous charging protocol. The black line is obtained analytically from Eq. (2.93). The red points correspond to experimental data, obtained from the *ibmq_toronto* machine. We have considered the same Gaussian pulse as in the qubit case with $t_m = 30$ ns. Image taken from [26].

close. Moreover, the charging occurs in roughly the same amount of time with respect to the other ($t_c \approx 20$ ns) with an analogous relaxation time ($t_c \approx 100$ μ s). It is worth to mention the fact that the departure from the theoretical curve is related to different sources of noise that lead to errors, including the initialization in the ground state, to discretization of pulses and the read-out errors.

Comparison with the state of the art

To conclude this Section about few levels QBs charged by a classical charger it is worth to make a comparison with state-of-the-art experiments. The most relevant result is the one reported in Ref. [24]. The authors of this work realized a three-level QB with a superconducting circuit in the transmon regime (see Section 1.2.3). They compared different charging protocols able to promote a qutrit from the ground state to a second excited state. In particular, they reasonably assume that the maximum admissible amplitude for the independently applied drives is bounded both at the level of the intensity or in modulus. Exactly saturating these bounds they have been able to apply the quantum brachistochrone theory [127] to obtain analytically solvable stable adiabatic charging protocols. Quantum brachistochrone theory provides the framework to determine the Hamiltonian that drives a quantum system between two states in the shortest physically allowed time, under given constraints on the available controls. In this setting, it allows one to identify time-optimal driving protocols, which in the present case lead to analytically solvable and stable adiabatic charging strategies. By controlling the sequence of these applied drives, they have been able to obtain either fast and unstable or slow and stable charging

processes, as shown in Fig. 2.6. In the former case the charging time is of the order of ≈ 100 ns, while in the latter case of ≈ 200 ns, namely two orders of magnitude shorter with respect to the typical relaxation and dephasing times of the considered device (≈ 20 μ s) and one order of magnitude longer than the one presented in this Section [26]. Concerning the energy, the maximum amount of energy that can be stored in this QB is $\mathcal{E}_{\max} = 51$ μ eV, comparable to the value of $\Delta_{\max}$ reported before.

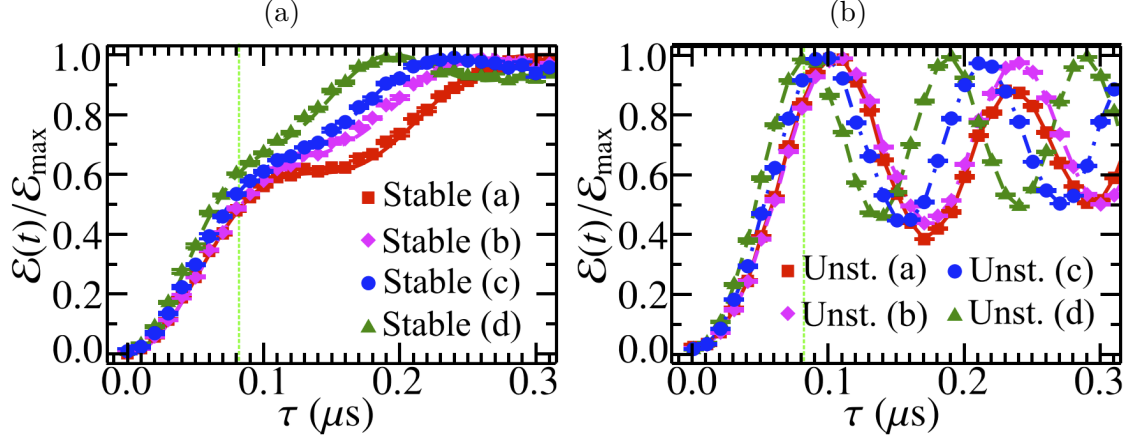


Figure 2.6: Experimental results of the ergotropy as a function of time, $\mathcal{E}(t)$, expressed in units of $\mathcal{E}_{\max} = 51$ μ eV for (a) stable and (b) unstable charging processes. Image adapted from [24] with minor modifications.

2.4 Dicke QB

We want now to describe a representative model of a QB with a quantum charger, the Dicke QB. It is given by a system where the energy of photons trapped into a resonant cavity (acting as the charger) is coherently transferred to a QB composed of N quantum units, namely a collection of identical independent TLSs. This model describes, for example, an ensemble of real or artificial atoms embedded in a Fabry-Perot cavity, namely a resonator consisting of two parallel, highly reflective mirrors placed a certain distance apart [128, 129].

In this system, the energy is initially stored into the cavity and flows towards the TLSs due to a proper modulation of the matter-radiation coupling [11]. In this framework, it is possible to study two opposite regimes: in the first one the TLSs are resonant with the cavity [10], namely they are characterized by the same typical energy, in the second one they are off-resonant [61], in particular we will address the case where the photons are way more energetic than the TLSs. The results of these works have been published in Refs. [61, 62] and the following Sections are largely based upon them.

2.4.1 The Dicke model

We consider a QB composed by N TLSs embedded into a resonant cavity that acts as a charger. The Hamiltonian describing the dynamics of this device, considered as

a closed system and assuming the conventional dipolar matter-radiation coupling, is [128]

$$\hat{\mathcal{H}}_D(t) = \omega_z \hat{J}_z + \omega_c \hat{a}^\dagger \hat{a} + 2\lambda(t) \hat{J}_x (\hat{a}^\dagger + \hat{a}), \quad (2.94)$$

with ω_z the energy of the TLSs (assumed identical), ω_c the one of the photons in the cavity, created (destroyed) by the operator $\hat{a}^\dagger$ ($\hat{a}$) and

$$\hat{J}_{x,z} = \frac{1}{2} \sum_{i=1}^N \hat{\sigma}_{x,z}^{(i)}, \quad (2.95)$$

the (pseudo)-spin operators with $\hat{\sigma}_{x,z}^{(i)}$ the conventional Pauli matrices associated to the i -th TLS as defined in Eq. (1.4). Moreover, we want to be able to turn on the matter-radiation coupling λ only for a tunable amount of time $\bar{t}$, we can assume

$$\lambda(t) = \lambda_0 \theta(t) \theta(\bar{t} - t). \quad (2.96)$$

with $\theta(t)$ the Heaviside step function. This kind of dynamics can be realized in the framework of quantum electrodynamics for example by introducing additional elements in the circuit which play the role of quantum couplers [130–132].

As anticipated, in the following, we will address two relevant operating regimes for the QB.

- i) *Resonant regime.* Here the energy of the TLSs is equal to the one of the photons, namely $\omega_c = \omega_z$. In this case the Hamiltonian in Eq. (2.94) becomes

$$\hat{\mathcal{H}}_D(t) \rightarrow \hat{\mathcal{H}}_D^{(R)}(t) = \omega_z \hat{J}_z + \omega_z \hat{a}^\dagger \hat{a} + 2\lambda(t) \hat{J}_x (\hat{a}^\dagger + \hat{a}). \quad (2.97)$$

This regime can be obtained in a superconducting circuit coupled with microwave radiation generated for example by means of an LC circuit [10].

- ii) *Off-resonant regime.* Here we consider the case of highly energetic photons ($\omega_c \gg \omega_z$) under dispersive conditions ($\omega_c - \omega_z \gg \lambda_0$) [61]. In this case, through Schrieffer-Wolff transformation [133], it is possible to derive an effective (infinite range) TLS-TLS interaction [134] leading to an Hamiltonian of the Lipkin–Meshkov–Glick (LMG) kind [135, 136] (see App. B.1 for more details about the transformation)

$$\hat{\mathcal{H}}_D(t) \rightarrow \hat{\mathcal{H}}_D^{(O)}(t) = \omega_z \hat{J}_z + \omega_c \hat{a}^\dagger \hat{a} - 4 \frac{\lambda^2(t)}{\omega_c} \hat{J}_x^2. \quad (2.98)$$

Higher order corrections in λ_0/ω_c lead to fast oscillations, which play only a minor role in the dynamics and can be neglected. This regime can be achieved through a coupling of the same qubits with infrared radiation.

We will characterize these two different operating regimes analyzing the scaling of their relevant figures of merit as a function of the number of TLSs N . In order to be able to make a fair comparison between the regimes, we will consider for both cases the same initial state at $t = 0$, namely

$$|\Psi(0)\rangle = |N\rangle \otimes |0, \dots, 0\rangle^{N \text{ TLSs}}, \quad (2.99)$$

where the first term of the tensor product represents a Fock state with N photons in the cavity, while the second term indicates that all the N TLSs are initially in the ground state $|0\rangle$. In the literature, other initial states have also been considered, such as coherent states for the photons in the cavity [11]. However, due to the form of $\hat{\mathcal{H}}_D^{(O)}$ in Eq. (2.98), it is worth to note that the photon part plays no role in the off-resonant case for the figures of merit we are going to discuss [26]. Moreover, notice that we will confine our analysis to a finite number of N photons. It is worth noting that in the thermodynamic limit ($N \gg 1$), the quantized mode can be effectively replaced by a classical monochromatic field; further details and a discussion on this correspondence are provided in App. B.2 [110].

2.4.2 Resonant regime

The first example of a QB based on the Dicke model found in literature operates in the resonant regime [10]. This configuration is particularly advantageous, as tuning the cavity and the TLSs to the same characteristic energy naturally promotes energy transfer from the cavity to the TLSs, effectively charging the QB. An additional benefit of this regime is that the interaction between the subsystems can be easily switched off by detuning the cavity. On the other hand, the critical challenge lies in experimentally holding the resonance condition throughout the charging process, as even small deviations can affect the efficiency and stability of the energy transfer. Once the system is charged, the interaction is turned off, leaving the TLSs in an excited state whose stability depends on their relaxation and dephasing times as anticipated in Section 1.2.4 [17, 25, 117, 127, 137, 138].

This kind of device displays a collective speed-up of the charging process. To make clear the advantage introduced by the Dicke QB, it is worth to compare two possible charging protocol. In Fig. 2.7 they are schematically shown: in panel (a), each TLS is coupled to a separate cavity, each hosting a single photonic mode, in this case we have a *parallel charging protocol*, in panel (b), an ensemble of many TLSs is embedded in a single cavity and interacting with a common photonic mode, in this case we have a *collective charging protocol*.

Parallel charging protocol

In this scenario, the Dicke Hamiltonian reduces to the Jaynes-Cummings Hamiltonian [139, 140]

$$\hat{\mathcal{H}}_R(t) = \omega_z \hat{\sigma}_z + \omega_c \hat{a}^\dagger \hat{a} + 2\lambda(t) \hat{\sigma}_x (\hat{a}^\dagger + \hat{a}). \quad (2.100)$$

It is possible to prove that [10]

$$E_B^{(\parallel)}(t) = N E^{(1)}(t) \quad (2.101)$$

with $E_B^{(\parallel)}(t)$ the energy stored at time t with the parallel charging protocol and $E_B^{(1)}(t)$ the energy stored in a single Rabi QB. As a consequence, looking at the maximum stored energy $E_{max}^{(\parallel)}$ and maximum average charging power $P_{max}^{(\parallel)}$, we get the following scaling laws

$$E_{max}^{(\parallel)} \propto N, \quad (2.102)$$

$$P_{max}^{(\parallel)} \propto N. \quad (2.103)$$

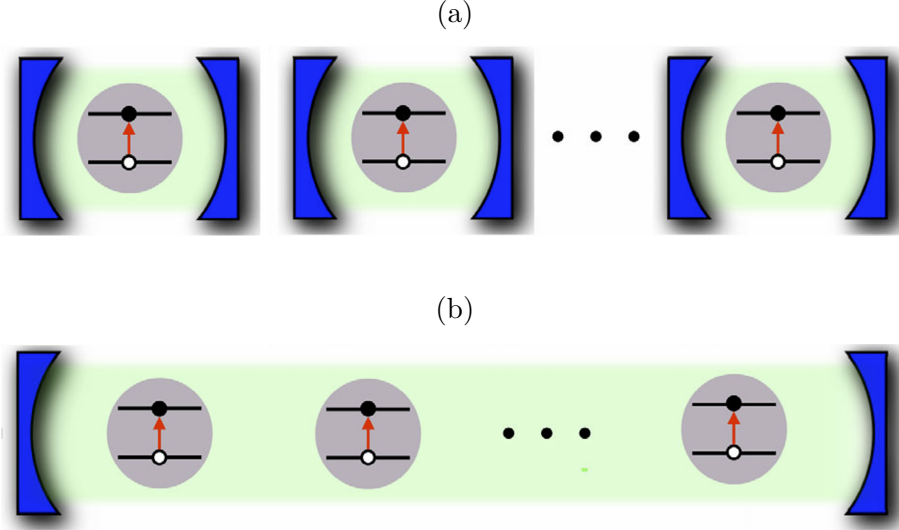


Figure 2.7: (a) An array of identical Rabi QBs operating in parallel. The elementary building block consists of a TLS with an energy separation ω_z between the ground $|0\rangle$ and excited state $|1\rangle$. Each TLS is coupled to a separate photonic cavity (blue). The red arrow indicates a particle-hole transition induced by the photon field. (b) A Dicke QB, where the same array of TLSs is embedded into a single cavity and interacting with a common photonic mode. Image taken from [10] and adapted.

Collective charging protocol

More interesting is the collective charging protocol. In Fig. 2.8 it is shown the maximum stored energy $E_{\max}^{(\#)}$ in units of $N\hbar\omega_c$ and the maximum averaged charging power $P_{\max}^{(\#)}$ in units of $N\sqrt{N}\hbar\omega_c$ as a function of the number of TLSs, N . We clearly

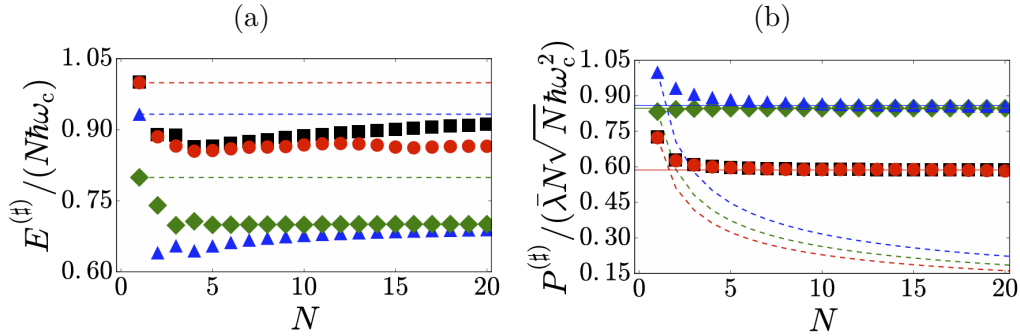


Figure 2.8: (a) Maximum stored energy $E_{\max}^{(\#)}$ (in units of $N\hbar\omega_c$) and (b) maximum averaged charging power $P_{\max}^{(\#)}$ (in units of $gN\sqrt{N}\hbar\omega_c$) as a function of the number of TLSs N . Black squares denote results for the Tavis Cummings model at $g/\omega_C = 0.05$. Results for Dicke QBs refer to $g/\omega_C = 0.05$ (red circles), $g/\omega_C = 0.5$ (blue triangles), and $g/\omega_C = 2$ (green diamonds). Image taken from [10] and adapted.

see that such rescaled quantities converge to an asymptotic value as N increases.

This implies the following scaling laws

$$E_{max}^{(\#)} \propto N, \quad (2.104)$$

$$P_{max}^{(\#)} \propto N^{\frac{3}{2}}. \quad (2.105)$$

This shows that in the collective regime the maximum charging power grows with a larger exponent than in the parallel case, highlighting the genuine advantage provided by collective quantum effects. As will be discussed in the following, this fact has attracted a great interest and a first step towards the realization of a Dicke QB has been experimentally implemented in an excitonic system made of fluorescent organic molecules dispersed in an inert matrix, where the Dicke superabsorption leads to a collective boost of the charging process [14, 108].

2.4.3 Off-resonant regime

Having demonstrated the super-extensive scaling of power in the resonant Dicke QB, it is natural to ask whether a similar advantage can be found in a different regime, one that may be easier to realize experimentally. As we will see in this Section, the answer is yes: a promising alternative is offered by the off-resonant regime [61].

In this case the charging is mediated by virtual photons and the cavity can be also empty. The two systems (charger and QB) are far detuned in energy, preventing any direct energy flow between them. This makes the systems easier to realize with respect to the resonant Dicke QB and allows us to describe it in the so-called dispersive regime, namely $\lambda_0 \ll |\omega_c - \omega_z|$. According to the analysis carried out in App. B.1, considering the Schrieffer–Wolff transformation [124] up to the second order in λ_0 and the condition of highly energetic photons $\omega_c \gg \omega_z$, we obtain the effective Hamiltonian $\hat{\mathcal{H}}_D^{(O)}$ in Eq. (2.98) [134].

The Hamiltonian in Eq. (2.98) is characterized by an effective infinite range interaction between the TLSs of the LMG kind [135, 136, 141] mediated by virtual photons playing the role of a quantum bus [142]. Here the quantum bus is an intermediate quantum degree of freedom, typically a field mode or a collective excitation, that mediates coherent interactions among otherwise non-interacting TLSs. By coupling each TLS to the same bus, the system acquires effective long-range interactions and can exchange excitations collectively. Such kind of infinite range interaction has been indicated as an ideal condition to achieve high power QBs [9, 27, 143].

To analyze the off-resonant regime it is useful to refer to two opposite limits, the weak coupling regime, when $g \ll \omega_z$ and the strong coupling regime with $g \sim \omega_z$, with $g = \frac{4\lambda^2}{\omega_c}$.

Weak coupling regime

In the weak coupling regime it is possible to derive analytical expressions for the energy stored and the average power using a time-dependent perturbative approach (see App. B.3 for more details about the derivation). This leads to

$$E_B^{(w)}(t) \approx \frac{g^2}{8} \frac{1 - \cos 2\omega_z t}{\omega_z} (N^2 - N), \quad (2.106)$$

and

$$P^{(w)}(t) \approx \frac{g^2}{8} \frac{1 - \cos 2\omega_z t}{\omega_z t} (N^2 - N). \quad (2.107)$$

Starting from Eq. (2.106) we obtain the values of the maximal stored energy and of the charging time associated with the first maximum, namely

$$E_{max}^{(w)} = \frac{g^2}{4\omega_z} (N^2 - N), \quad (2.108)$$

$$\omega_z t_E = \frac{\pi}{2}, \quad (2.109)$$

respectively. Analogously for the averaged charging power in Eq. (2.107) we have

$$P_{max}^{(w)} \approx \frac{g^2}{4.46} (N^2 - N), \quad (2.110)$$

$$\omega_z t_P \approx 1.16, \quad (2.111)$$

where the values in this case need to be extracted numerically. Fig. 2.9 shows the scalings of maximum stored energy and maximum power in units of $N\omega_z$ and $N\omega_z^2$ respectively and as a function of the number of TLSs N . This implies the following

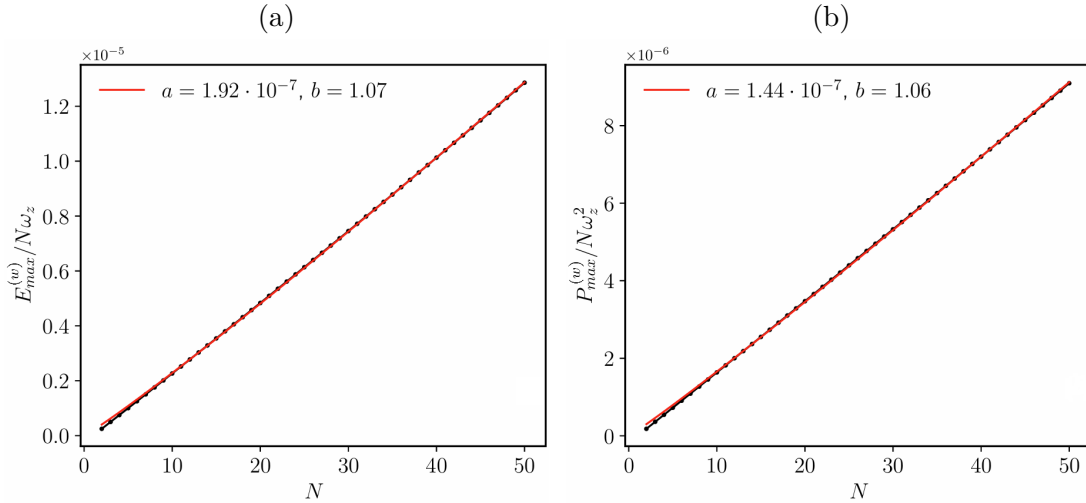


Figure 2.9: (a) Maximum stored energy $E_{max}^{(w)}$ (in units of $N\omega_z$) and (b) maximum averaged charging power $P_{max}^{(w)}$ (in units of $N\omega_z^2$) as a function of the number of TLSs N . In both panels $g = 10^{-3}\omega_z$. (b) Red curves are the fits of the numerical points according to: $E_{max}/N\omega_z = aN^b$ and $P_{max}/N\omega_z^2 = aN^b$. The values of the fitting parameters are indicated in the labels of each panel. Image taken from [61] with minor modifications.

scaling laws

$$E_{max}^{(w)} \propto N^2, \quad (2.112)$$

$$P_{max}^{(w)} \propto N^2. \quad (2.113)$$

Despite this very good scaling, even faster than the one achieve thought the collective charging protocol in the resonant regime, it must be pointed out that the absolute values of $E_{max}^{(w)}/N\omega_z$ and $P_{max}^{(w)}/N\omega_z^2$ are incredibly small.

Strong coupling

We can now investigate the strong coupling regime, namely a situation in which g is of the same order of ω_z [144]. In this regime, the first maximum of the energy stored into the QB is only a local maximum, with higher values of the energy possibly appearing at greater times. However, in the following we focus on it due to the fact that it is associated to a greater value of the power. In this regime, the charging of the QB can exceed the 50% near the maxima. According to a full numerical analysis, it is possible to deduce the scaling behaviour of the various figures of merit in the strong coupling regime as shown in Fig. 2.10,

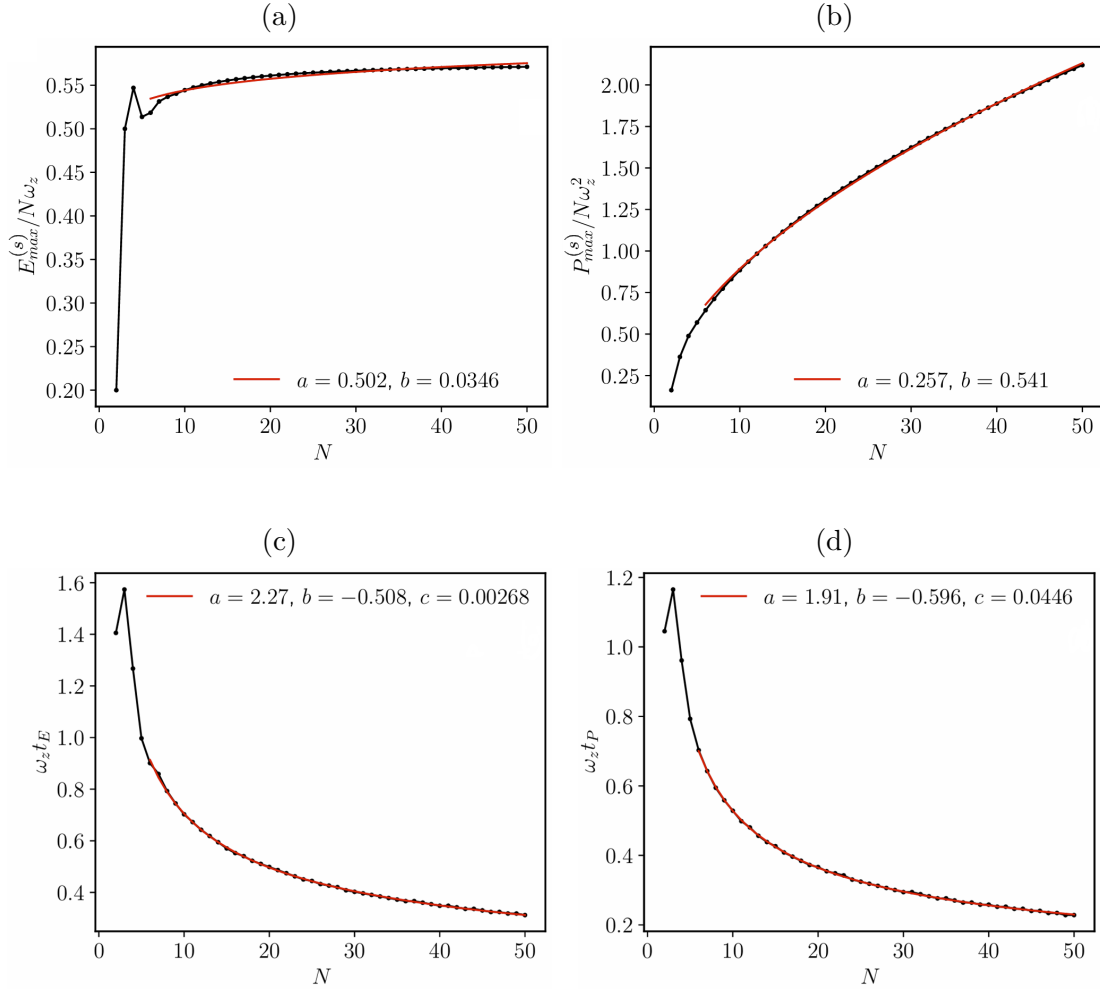


Figure 2.10: (a) Maximum stored energy $E_{\max}^{(s)}$ (in units of $N\omega_z$) and (c) corresponding charging time $\omega_z t_E$ as a function of the number of TLSs N . (b) Maximum averaged charging power $P_{\max}^{(s)}$ (in units of $N\omega_z^2$) and (d) corresponding charging time $\omega_z t_P$ as a function of the number of TLSs N . In both panels $g = \omega_z$. Red curves are the fits of the numerical points according to: $E_{\max}^{(s)}/N\omega_z = aN^b$ (a), $P_{\max}^{(s)}/N\omega_z^2 = aN^b$ (b). The values of the fitting parameters are indicated in the labels of each panel. Image taken from [61] with minor modifications.

$$E_{max}^{(s)} \propto N, \quad (2.114)$$

$$P_{max}^{(s)} \propto N^{\frac{3}{2}}. \quad (2.115)$$

Notice that these are equal to the ones reported for the resonant regime described in the previous Section [10]. It is also worth to note that, even if difficult to be realized in the dissipative Dicke model with dipolar coupling, this situation could be reached by exploiting more exotic matter-radiation couplings such as the two-photon interaction and properly changing the initial photon distribution in the cavity (see App. B.1.3 for more details).

Considerations about universality

The two previous Paragraphs revealed two distinct scaling behaviors of the considered quantities under the two coupling regimes studied: the weak coupling regime exhibits better scaling with N , while the strong coupling regime appears more promising in terms of absolute values of energy storage, charging power, and ergotropy.

This change of behavior can be seen as a consequence of the Excited State Quantum Phase Transition (ESQPT) shown by both the Dicke and the effective LMG model (see Ref. [145] for a review on the subject). This represents the footprint of a quantum phase transition at the level of the excited states of the system. Its role in the present QB is justified by the fact that it is initialized in the ground state and charged by means of a protocol which naturally involves the excited states. In order to better clarify this point, we can consider the evolution of E_{max} as a function of the renormalized coupling $G = gN$ (see Fig. 2.11). The choice of this renormalized parameter to characterize the evolution of the system can be justified by considering the classical limit of the effective LMG model (see App. B.2 for more details) and is reminiscent of the renormalization $g\sqrt{N}$ observed for the Dicke model [10]. Notice that the emergence of a crossover behaviour for the maximum stored energy is motivated by the fact that it is closely related to the order parameter of the system, namely the total magnetization, which at a given time t can be written as

$$\mathcal{M}(t) = \langle \psi(t) | \hat{J}_z | \psi(t) \rangle = \frac{E_B(t)}{\omega_z} + \langle \psi(0) | \hat{J}_z | \psi(0) \rangle. \quad (2.116)$$

It is possible to observe now two different regimes for $G < \omega_z$ and $G > \omega_z$ respectively, with a crossover in correspondence of the ESQPT of the model, occurring at $G = \omega_z$. Incidentally, by increasing the value of G (Fig. 2.11(b)) one has that the maximum value of energy per TLS reachable in the considered QB can exceed, the 60%. Remarkably enough, this value is compatible with what is observed for the Dicke model in the strong coupling regime and under resonant conditions [10]. This makes the off-resonant Dicke QB competitive for practical experimental realizations, also taking into account the fact that it can be realized also using a vacuum cavity, where the electromagnetic mode is kept in its ground state $|0\rangle$. Such a configuration is easier to engineer and more stable compared to the resonant Dicke QB, as it relies solely on vacuum fluctuations rather than requiring the preparation of specific photonic states. Moreover, the dependence on the renormalized coupling G allows to extend the validity of the previous analysis carried out for the strong coupling regime by increasing the number of TLS composing the QB.

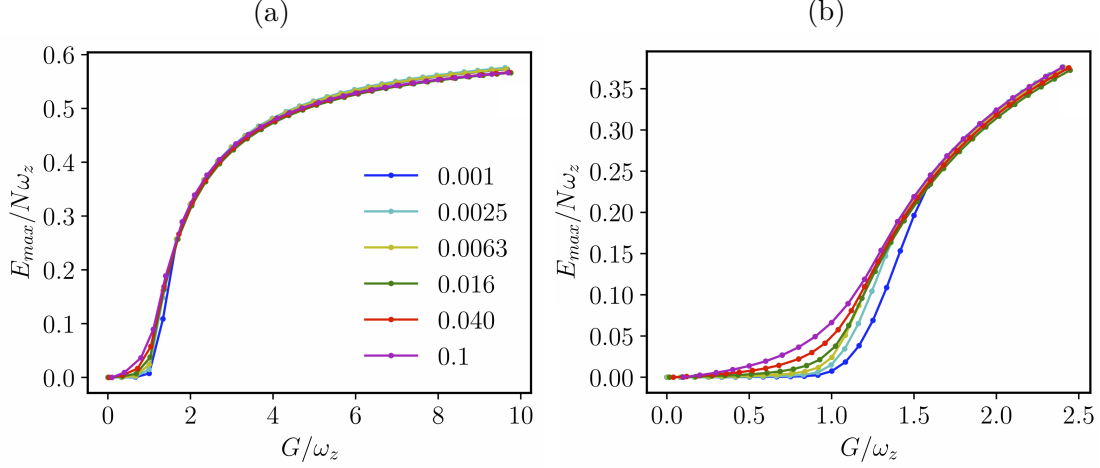


Figure 2.11: (a) Behaviour of E_{max} (in units of $N\omega_z$) as a function of the rescaled coupling $G = gN$ (in units of ω_z) for various values of g and (b) its zoom around the crossover at $G = \omega_z$. Values of the coupling are reported in the color scale of the legend. Image taken from [61].

2.4.4 Consideration about ergotropy

We will finally give some details about the local ergotropy, namely the work that can be extracted by addressing separately the TLSs composing the QB, as anticipated in Section 2.2.3.

We can consider the 2×2 reduced density matrix $\hat{\rho}_B^{(1)}$, describing the first TLS at a given instant while the energy is measured with respect to the Hamiltonian

$$\hat{h}_B^{(1)} = \frac{\omega_z}{2} \hat{\sigma}_z^{(1)}. \quad (2.117)$$

Notice that, due to the invariance under TLSs permutations of the Hamiltonian in Eq. (2.94), we can focus on the first TLS without any loss of generality. Thus, the maximum energy that can be extracted from a single battery unit in an N TLSs device is given by

$$\mathcal{E}_l^{(1)}(t) \equiv \mathcal{E}(\hat{\rho}_B^{(1)}(t), \hat{h}_B^{(1)}) . \quad (2.118)$$

Consistently with what is done above, this expression can be simplified by writing $\hat{\rho}_B^{(1)}(t)$ in the diagonal basis,

$$\hat{\rho}_B^{(1)}(t) = r_0(t)|r_0(t)\rangle\langle r_0(t)| + r_1(t)|r_1(t)\rangle\langle r_1(t)| , \quad (2.119)$$

where $r_0(t) \geq r_1(t)$. In this case, the ergotropy $\mathcal{E}_l^{(1)}(t)$ reduces to

$$\mathcal{E}_l^{(1)}(t) = \frac{E_B(t)}{N} - r_1(t)\omega_z , \quad (2.120)$$

where we used the fact that $\text{Tr}[\hat{\rho}_B^{(1)}(t)\hat{h}_B^{(1)}] = (E_B(t)/N)$ due to permutation symmetry. We have evaluated the above expression numerically, further details about this analysis can be found in Ref. [146].

Fig. 2.12 shows the time evolution of the energy stored in the QB and of the ergotropy of a single TLS (in units of $N\omega_z$), both in the weak and in the strong coupling regimes. Note that the latter is non-zero only if the former is greater than 0.5.

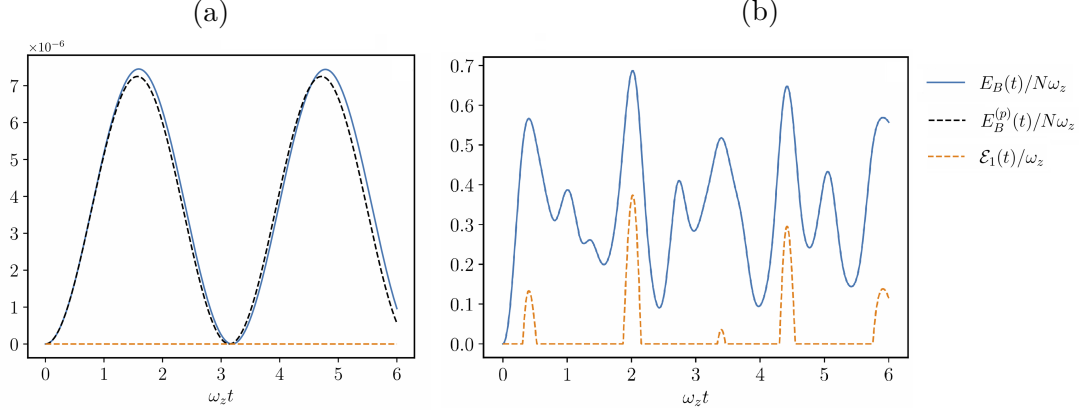


Figure 2.12: Energy stored into the QB $E_B(t)$ (in units of $N\omega_z$) and single TLS ergotropy $\mathcal{E}_1(t)$ (in units of ω_z) as a function of time (in units of ω_z^{-1}) for $N = 30$ and $\omega_z \bar{t} > 2\pi$. (a) Weak coupling regime, $g = 10^{-3}\omega_z$. Black curves represent the theoretical curves obtained through time-dependent perturbative expansions (indicated with the superscript p in the labels) in Eqs. (2.106). (b) Strong coupling regime, $g = \omega_z$. Image taken from [61] and adapted.

2.4.5 Experimental realization

At the beginning of 2022, the first experimental evidence of a QB was reported, consisting of fluorescent molecules embedded into a resonant cavity [14]. Given the energy level configuration of these molecules, approximable as TLSs, it was possible to carry out the experiment at room temperature. The role of the charger is played by an external laser and the intensity of the matter-radiation interaction is controlled by adjusting the density of the molecules in the cavity. This tuning let to have a transition from a dissipation-dominated regime to the resonant Dicke regime, described in Section 2.4.2. With this experiment it has been possible to observe a super-extensive scaling of the power ($P_{max} \propto N^{\frac{3}{2}}$). The stored energy per molecule is of the order of a fraction of electronVolt; however, charging and discharging occur on extremely short timescales (in the picosecond range), making the precise control of such kind of device a significant challenge.

The structures fabricated consist of a thin (active) layer of a low-mass molecular semiconductor dispersed into a polymer matrix that is deposited by spin coating and positioned between two dielectric mirrors, forming a microcavity as illustrated schematically in panel 2.13(a). Charging and energy storage dynamics were measured using ultrafast transient-absorption spectroscopy, allowing femtosecond charging times to be measured. Using this technique, authors excite the microcavity with a pump pulse and then measure the evolution of stored energy with a second probe pulse, delayed by time t (panel 2.13(b)). The experimental dynamics can be reproduced by modeling, with the Lindblad master equation [147, 148], the N TLSs in an optical cavity with light-matter coupling strength g , a driving laser with a Gaussian pulse envelope and peak amplitude η_0 , and three decay channels corresponding to the cavity decay (k), TLS dephasing (γ_z), and TLS relaxation (γ^-). Panel 2.13(c) shows the theoretical model with the experimental results in the three operating regimes. Measurements at different molecular concentrations

were performed, adjusting the pump fluence to maintain an approximately constant photon density (pump photons per molecule) $r = kN_\gamma/N$, where N is the total number of molecules in the excitation volume, N_γ is the total number of pump laser photons, and k is the fraction of them that actually reaches the active layer of the microcavity.

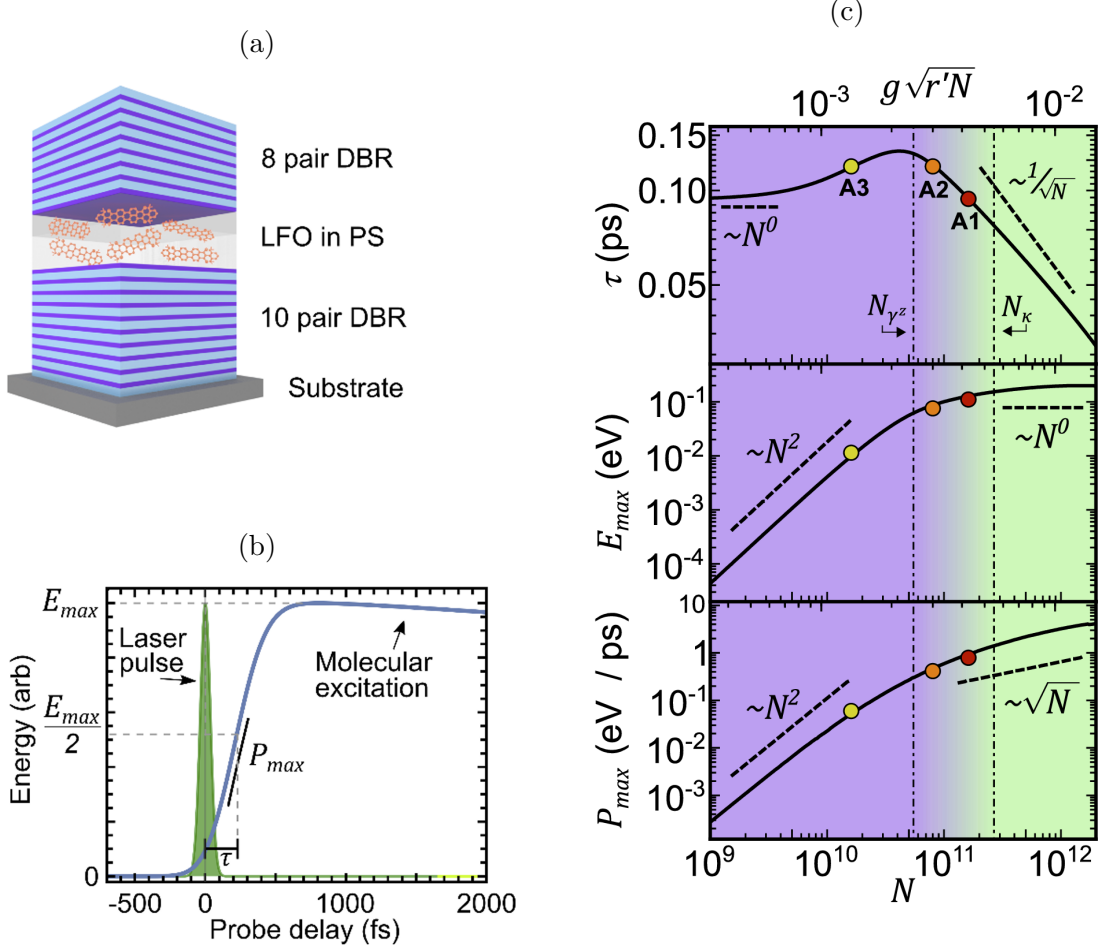


Figure 2.13: (a) Microcavity consisting of Lumogen-F Orange (LFO) dispersed in a polystyrene matrix (PS) between distributed Bragg reflectors (DBR). (b) A laser pump pulse excites the LFO molecules. The energy of the molecules are then measured with probe pulses delayed by time t , from which it is possible to ascertain the peak energy density (E_{max}), rise time (τ), and peak charging power (P_{max}). (c) Theoretical model (solid line) with three operating regimes: decay-dominated (purple), coupling-dominated (green), and a decay-coupling-crossover regime. The decay-dominated regime is bounded by $N_k < k^2/g^2r'$, and the coupling-dominated regime is bounded by $N_{\gamma z} > \gamma^2/g^2r'$, where $r' = 1$. The coloured dots indicate where the experiments sit on these curves. The uncertainty in N is 10%, which is smaller than the dot size. Image taken from [14] and adapted.

Recently new experiments have been realized with the aim of overcoming technical issues [37, 108]. One [37] promising strategy involves extending the energy storage lifetime of Dicke QBs by exploiting molecular triplet states within multi-layer microcavities, as demonstrated through the fabrication and characterization

of five devices tuned across a triplet-polariton resonance. The other [108] introduces a scalable method to induce steady-state superradiance in OLEDs, marking a significant advancement in the practical implementation of quantum optical effects in solid-state devices, closely related to what needed for QB. By engineering emitter-cavity interactions, the study demonstrates how quantum coherence can be harnessed to simultaneously enhance brightness, reduce power consumption, and improve spectral purity-key metrics for future high-performance optoelectronics.

Chapter 3

Cyclic solid-state quantum battery

The theoretical and experimental works presented in the previous Chapter mainly considered the energy stored in the QB and the associated charging power [11]. Despite their relevance for the advancement of the subject, it can be interesting to consider a more complete thermodynamic description of the operating regimes of these devices. An interesting strategy to do this consists in considering the operation of the QB as a thermodynamic cycle [114, 149]. In this framework, the QB coupled to its charger is first typically initialized in a thermal state. Then the QB is disconnected from the charger (involving some energy cost). During the next step, the ergotropy is taken out from the QB. The energy extraction in this configuration is guaranteed by the fact that a thermalized state for the whole system (QB+charger) is not, in general, a passive thermal state for the QB only. In the final stage of the cycle, the QB and the charger are connected again (involving, in principle, an additional energy cost) and the whole system is finally reinitialized, ready to perform a new cycle. In the original proposals [114, 149], the charger was assumed as a large system playing also the role of thermal bath (reservoir). This aspect may pose a challenge when implementing the protocols, as it is not always straightforward in practice to control the connection or disconnection of a quantum system from its environment. In this regard, it has also been recently shown that locally extracting work from a system in the presence of Hamiltonian couplings, for example with an environment, can deliver higher net work with respect to analogous protocols in which the interaction is switched off [150–153].

The aim of this Chapter is to introduce a cyclic QB model, based on an interacting bipartite system, weakly coupled to a thermal bath, but with the assumption that the operations are carried out on timescales shorter than those of thermalization as well as relaxation and dephasing of the QB. This ensures that the only role played by the bath is to reinitialize the system to the same thermal state at the end of each cycle. The results of this work have been published in Ref. [22], and the Chapter is largely based upon it.

3.1 Thermodynamic cycle

We consider here a bipartite interacting system of the form

$$\hat{\mathcal{H}}(t) = \hat{\mathcal{H}}_A + \hat{\mathcal{H}}_B + \hat{\mathcal{H}}_{\text{int}}(t) \equiv \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{int}}(t), \quad (3.1)$$

where $\hat{\mathcal{H}}_k$ denotes the local Hamiltonian of the k -th subsystem, $k = A, B$, and $\hat{\mathcal{H}}_{\text{int}}(t)$ the interaction between the two, that is external modulated in time. We model the time dependency as a Heaviside step function, $\hat{\mathcal{H}}_{\text{int}}(t) \propto \theta(\bar{t} - t)$ so that the interaction is finite and constant before $\bar{t}$ and zero after $\bar{t}$, modeling an instantaneous switching off (disconnection of the two subsystems). Moreover, we denote by ϱ the density matrix of the bipartite system and by ρ_k the reduced density matrix of the k -th subsystem. As anticipated, we assume to operate the working cycle while keeping the QB weakly coupled to a thermal bath at inverse temperature β . Note that the constant presence of a weakly coupled reservoir has a twofold motivation: first, it allows us to neglect the explicit contribution of the reservoir during the connection/disconnection and work extraction strokes; second, it makes unnecessary fully isolating the battery from the external environment. Therefore, this assumption appears as well-suited to describe a realistic scenario.

The interacting bipartite system is initialized in the thermal state τ_β , as defined in Eq. (2.29), at a time $t_0 < \bar{t}$. The interaction is then switched off at time $\bar{t}$, instantaneously disconnecting the two subsystems. After this operation, provided that the state τ_β is not passive with respect to the Hamiltonian $\hat{\mathcal{H}}_0$, it is possible to extract ergotropy from the systems. Section 3.1.1 will describe three possible protocols to perform this operation.

We now turn to the description of the four strokes of the working cycle of the cyclic QB. The cycle is sketched in Fig. 3.1. Starting from the bipartite system in a Gibbs state $\varrho_{\text{I}} = \tau_\beta$ reported in Eq. (2.29) with $\hat{\mathcal{H}}$ the Hamiltonian in Eq. (3.1), the following strokes are performed.

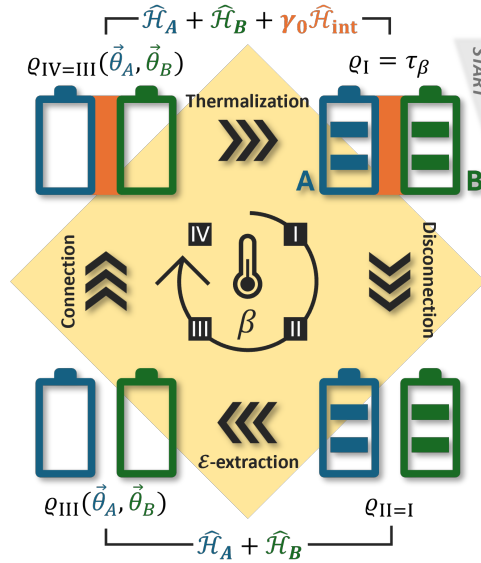


Figure 3.1: Working cycle of the bipartite cyclic QB. The bipartite system is initially (I) prepared in a Gibbs state τ_β reported in Eq. (2.29) at inverse temperature β . (I $\rightarrow$ II) Disconnection of subsystems (switching off of $\hat{\mathcal{H}}_{\text{int}}$); (II $\rightarrow$ III) Ergotropy extraction from the system (pictorially represented as an empty battery); (III $\rightarrow$ IV) Connection of subsystems (switching on of $\hat{\mathcal{H}}_{\text{int}}$); (IV $\rightarrow$ I) Thermalization to restore the initial Gibbs state and restart the cycle. Throughout the whole cycle, the bipartite system is weakly coupled to a thermal reservoir at inverse temperature β (pictorially represented by the yellow shaded area). Image taken from [22].

(I $\rightarrow$ II) *Disconnection of subsystems.* It is accomplished by switching off the

interaction. After disconnection, the system is in the state $\varrho_{\text{II}} = \varrho_{\text{I}}$, since this instantaneous stroke leaves the state unchanged. Therefore, the energy cost for this stroke reads

$$E_d = -\text{Tr}\left[\hat{\mathcal{H}}_{\text{int}}\varrho_{\text{I}}\right], \quad (3.2)$$

and is independent of the protocol considered for extracting work.

(II→III) *Extraction of ergotropy.* It is accomplished by performing a cyclic unitary operation $\hat{\mathcal{U}}_p$ on the state ϱ_{II} , leading to $\varrho_{\text{III}}^{(p)}(\theta) = \hat{\mathcal{U}}_p(\theta)\varrho_{\text{II}}\hat{\mathcal{U}}_p^\dagger(\theta)$, where the subscript p refers to the protocol used to extract the ergotropy, that will be discussed in the following, and θ denotes a possible arbitrary phases, if any. The amount of extracted work and the associated unitary, hence also the final state, depend on the chosen protocol and therefore it will be defined in Section 3.1.1 and evaluated in Section 3.2. The possible presence of arbitrary phases will affect the result of the next stroke.

(III→IV) *Connection of subsystems.* It is accomplished by switching on the interaction. After connection, the system is in the state $\varrho_{\text{IV}}^{(p)}(\theta) = \varrho_{\text{III}}^{(p)}(\theta)$, since this instantaneous stroke leaves the state unchanged. Therefore, the energy cost for this stroke reads

$$E_c^{(p)}(\theta) = \text{Tr}\left[\hat{\mathcal{H}}_{\text{int}}\varrho_{\text{III}}^{(p)}(\theta)\right]. \quad (3.3)$$

(IV→I) *Thermalization.* The bipartite system is always in contact with an external thermal reservoir (weak coupling) throughout the whole cycle. During this last stroke, the system is left to naturally thermalize. This restores the initial thermal state at a vanishing energetic cost. In other words, this stroke can be intended as the process of recharging of the battery.

After describing this working cycle energetics, we define its efficiency as the ratio between the energy delivered by the battery and the energy cost to run the cycle [114, 149]

$$\eta^{(p)}(\theta) = \frac{\mathcal{E}^{(p)}}{E_d + E_c^{(p)}(\theta)}, \quad (3.4)$$

with $0 \leq \eta^{(p)}(\theta) \leq 1$. These bounds are explained as follows. The net result of the strokes (I→...→IV) is a unitary evolution of the bipartite system, $\varrho_{\text{I}} \rightarrow \varrho_{\text{IV}}^{(p)}(\theta)$, and an associated cyclic change of the total Hamiltonian, with $\hat{\mathcal{H}}^{(\text{I})} = \hat{\mathcal{H}}^{(\text{IV})} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{int}}$ and $\hat{\mathcal{H}}^{(\text{II})} = \hat{\mathcal{H}}^{(\text{III})} = \hat{\mathcal{H}}_0$. Hence, the initial passive state can only increase its average energy,

$$\text{Tr}\left[\hat{\mathcal{H}}(\varrho_{\text{IV}}^{(p)}(\theta) - \varrho_{\text{I}})\right] \geq 0, \quad (3.5)$$

and this increase must be equal to the non-negative work

$$E_d - \mathcal{E}^{(p)} + E_c^{(p)}(\theta) \geq 0 \quad (3.6)$$

performed on the system during the strokes (I→...→IV). The bounds on the efficiency follow accordingly, being $\mathcal{E}^{(p)} \geq 0$ by definition, and $E_d + E_c^{(p)}(\theta) \geq \mathcal{E}^{(p)}$.

The following Section is dedicated to the description of the three protocols that we have studied to extract the ergotropy.

3.1.1 Ergotropy extraction

Denoting by $\mathcal{E}^{(p)}$ the ergotropy extracted by the generic protocol p , we introduce the following protocols.

Protocol (i) ($p = s$). The resource consists of a single subsystem, say A . The extractable work $\mathcal{E}^{(s)} = \mathcal{E}_A$ is the ergotropy of the subsystem A . The process which accomplishes this task is the unitary

$$\hat{\mathcal{U}}_s(\boldsymbol{\theta}_A) = \hat{U}_A(\boldsymbol{\theta}_A) \otimes \hat{I}_B. \quad (3.7)$$

The main reason for processing just one subsystem is the interest in managing energy locally.¹ To recall that in this protocol the resource is a single subsystem, we address it with $p = s$.

Protocol (ii) ($p = l$). The resource consists of both subsystems, A and B , separately. The extractable work $\mathcal{E}^{(l)} = \mathcal{E}_A + \mathcal{E}_B$ is the local ergotropy. The process which accomplishes this task is the local unitary operations

$$\hat{\mathcal{U}}_l(\boldsymbol{\theta}_A, \boldsymbol{\theta}_B) = \hat{U}_A(\boldsymbol{\theta}_A) \otimes \hat{U}_B(\boldsymbol{\theta}_B). \quad (3.8)$$

To recall that in this protocol the ergotropy is extracted with local unitary operations, we address it with $p = l$.

Protocol (iii) ($p = g$). The resource consists of both subsystems, A and B , including correlations. The extractable work $\mathcal{E}^{(g)}$ is the global ergotropy in Eq. (2.118). The process which accomplishes this task is the global unitary $\hat{\mathcal{U}}_g$ defined as in Eq. (2.17). Note that this is possible because τ_β is completely passive with respect to the Hamiltonian in Eq. (3.1) with $\theta(\bar{t} - t) = 1$, but can be active with respect to $\hat{\mathcal{H}}_0 = \hat{\mathcal{H}}_A + \hat{\mathcal{H}}_B$, which is the Hamiltonian of the bipartite system after disconnection. In this case, no arbitrary phases are included in the unitary, because irrelevant. To recall that in this protocol the ergotropy is extracted with a global unitary operation, we address it with $p = g$.

Following the definition in Eq. (2.19), the maximum work that can be extracted by a unitary of the form in Eq. (3.8) is referred to as *local ergotropy* [154–156] and reads

$$\begin{aligned} \mathcal{E}^{(l)} &\equiv \text{Tr} \left[(\hat{\mathcal{H}}_A + \hat{\mathcal{H}}_B) \left(\varrho - \pi_l(\boldsymbol{\theta}_A, \boldsymbol{\theta}_B) \right) \right] \\ &= \text{Tr} \left[\hat{\mathcal{H}}_A (\rho_A - \pi_A) \right] + \text{Tr} \left[\hat{\mathcal{H}}_B (\rho_B - \pi_B) \right] \\ &= \mathcal{E}_A + \mathcal{E}_B \geq 0, \end{aligned} \quad (3.9)$$

where

$$\pi_l(\boldsymbol{\theta}_A, \boldsymbol{\theta}_B) = \hat{\mathcal{U}}_l(\boldsymbol{\theta}_A, \boldsymbol{\theta}_B) \tau_\beta \hat{\mathcal{U}}_l^\dagger(\boldsymbol{\theta}_A, \boldsymbol{\theta}_B). \quad (3.10)$$

Note that the state in Eq. (3.10) is not the product state $\pi_l \neq \pi_A \otimes \pi_B$, in general, because correlations are preserved by local unitary transformations. Moreover, the state $\pi_l(\boldsymbol{\theta}_A, \boldsymbol{\theta}_B)$ is not necessarily passive with respect to $\hat{\mathcal{H}}_A + \hat{\mathcal{H}}_B$, because ergotropy has been extracted locally, not globally. Indeed, the passive state of τ_β with respect to $\hat{\mathcal{H}}_A + \hat{\mathcal{H}}_B$ is $\pi_g = \hat{\mathcal{U}}_g \tau_\beta \hat{\mathcal{U}}_g^\dagger$.

¹We also mention as a possible reason the case in which the reduced state of subsystem B is already passive with respect to $\hat{\mathcal{H}}_B$, $\text{Tr}_A[\tau_\beta] = \pi_B$. This happens, e.g., for two interacting qubits with Hamiltonian $\hat{\mathcal{H}} = \Omega_A \hat{\sigma}_A^z + \Omega_B \hat{\sigma}_B^z + \gamma_0 \hat{\sigma}_A^z \otimes \hat{\sigma}_B^z$ —where $\Omega_B = 2\Omega_A > 0$, $\gamma_0 = 1.5\Omega_A$, and $\beta = 2/\Omega_A$ —prepared in the thermal state τ_β . The reduced state $\rho_{A(B)} = \text{Tr}_{B(A)}[\tau_\beta]$ is active (passive) with respect to the local Hamiltonian $\hat{\mathcal{H}}_{A(B)}$.

In the following, in order to avoid confusion, we will explicitly refer to the ergotropy defined in Eq. (2.118) as *global* ergotropy, denoting by $\mathcal{E}^{(g)}$. If it is extracted by a global unitary $\hat{U}_g$ acting on the overall system, the inequality $\mathcal{E}^{(l)} \leq \mathcal{E}^{(g)}$ holds, because as we anticipated in Section 2.2.3, the global unitary can extract work also from correlations, while the local unitaries only from the subsystems.

In the following Sections, we theoretically describe a system based on superconducting circuits where the working cycle discussed above can be implemented in practice. Starting from that model, we compare the performance of the proposed model of cyclic QB depending on the adopted protocols (i)–(iii) described above. After studying the ideal scenario, we simulate Protocol (i), $p = s$, ergotropy extracted from a single subsystem, on an IBM quantum computer.

3.2 Energetics of the working cycle of the QB

In order to proceed further with the analysis of the system, it is now necessary to specify the explicit form of the Hamiltonian that we want to study. We consider a setup based on three symmetrical dc-superconducting quantum interference devices (dc-SQUID)s, the bipartite QB comprises the first two dc-SQUIDS, while the third one plays the role of a tunable quantum coupler between them [130–132].

The proposed circuit and the derivation of the Hamiltonian is reported in App. C.1, and we find a Josephson QB (JQB) with Hamiltonian

$$\begin{aligned}\hat{\mathcal{H}}(t) &= \Omega[\hat{\sigma}_A^z + \hat{\sigma}_B^z] - \Omega\gamma(t)(\hat{\sigma}_A^x + \hat{\sigma}_B^x + \hat{\sigma}_A^x\hat{\sigma}_B^x - \hat{\sigma}_A^y\hat{\sigma}_B^y) \\ &\equiv \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{int}}(t),\end{aligned}\tag{3.11}$$

where we have identified the Hamiltonians $\hat{\mathcal{H}}_0$ and $\hat{\mathcal{H}}_{\text{int}}(t)$ with $\gamma(t) = \theta(\bar{t} - t)\gamma_0$ and $\gamma_0 \neq 0$. Notice that $\hat{\mathcal{H}}_{\text{int}}(t)$ includes single-qubit terms, in addition to the two-qubit interaction. In the following we will omit Ω , the reference scale for the energies.

We can now study the cycle described in Section 3.1, for all the three protocols $p = s, l, g$ for extracting work. We recall that the external driving of our model, ultimately the magnetic flux, not only affects the interaction between qubits but also the local Hamiltonian of each qubit.

After the instantaneous disconnection, the local Hamiltonian of the k -th qubit is just $\hat{\mathcal{H}}_k = \hat{\sigma}_k^z$. The reduced state of the qubit is $\rho_{A(B),\text{II}} = \text{Tr}_{B(A)}[\tau_\beta]$. Notice that, since the two qubits are identical and the thermal state τ_β is symmetric under exchange of the two qubits (symmetry inherited from the Hamiltonian in Eq. (3.11)), the reduced states of the qubits are equal, $\rho_{k,\text{II}} \equiv \rho_{\text{II}}$.

Following the analysis in Section 2.2.3, we have already proved that the unitary operation needed to extract ergotropy from a qubit is the one in Eq. (2.27). Notice that, in that equation, we have explicitly taken into account that $r_y = 0$. This is true due to the fact that the Gibbs state, and so ρ_{II} , is a real density matrix. The passive state of the qubit with respect to $\hat{\sigma}_z$, the spectrum of the latter being non-degenerate, is unique $\rho_{\text{III}} = \hat{U}(\theta)\rho_{\text{II}}\hat{U}^\dagger(\theta) = \frac{1}{2}(1 - r\hat{\sigma}_z)$, independent of θ , and thermal, being it a TLS [60], at an effective inverse temperature $\beta_{\text{eff}} = \text{arctanh}(r)$. A unitary transformation preserves the purity of a state, thus both ρ_{II} and ρ_{III} have the same r . From this qubit, the ergotropy extracted by the unitary operation in Eq. (2.27) is

$$\mathcal{E} = r_z + r = \langle \hat{\sigma}_A^z \rangle + \sqrt{\langle \hat{\sigma}_A^x \rangle^2 + \langle \hat{\sigma}_A^y \rangle^2}.\tag{3.12}$$

Now, we analytically inspect the energetics of the strokes in the working cycle based on the extraction of the ergotropy $\mathcal{E}^{(s)}$ from the single qubit [Protocol (i)], of the local ergotropy $\mathcal{E}^{(l)}$ from both the qubits [Protocol (ii)], and of the global ergotropy $\mathcal{E}^{(g)}$ [Protocol (iii)] from both the qubits, including correlations. Deferring all the details to App. C.2, here we quote only the final results. For all three considered scenarios, the energy cost for disconnection, defined in Eq. (3.2), is

$$E_d = \gamma_0(2\langle\hat{\sigma}_A^x\rangle + \langle\hat{\sigma}_A^x\hat{\sigma}_B^x\rangle - \langle\hat{\sigma}_A^y\hat{\sigma}_B^y\rangle). \quad (3.13)$$

The work, instead, differs: for $p = s$ we have $\mathcal{E}^{(s)} = \mathcal{E}$ in Eq. (3.12) extracted by $\hat{\mathcal{U}}_s(\theta)$ in Eq. (3.7), and for $p = l$ we have $\mathcal{E}^{(l)} = 2\mathcal{E}$ by $\hat{\mathcal{U}}_l(\theta_A, \theta_B)$ in Eq. (3.8), where the single-qubit unitary is given in Eq. (2.27). Moreover, for $p = g$, the global ergotropy is extracted by $\hat{\mathcal{U}}_g$, reported in Eq. (2.17), and reads

$$\mathcal{E}^{(g)} = 2\langle\hat{\sigma}_A^z\rangle + \frac{2}{\text{Tr}[e^{-\beta\hat{\mathcal{H}}}]}\left(e^{-\beta\epsilon_1} - e^{-\beta\epsilon_4}\right) \geq \mathcal{E}^{(l)}, \quad (3.14)$$

where ϵ_1 and ϵ_4 are, respectively, the lowest and the highest energy level of $\hat{\mathcal{H}}$ in Eq. (3.11) with $\gamma(t) = \gamma_0$ (see App. C.2.3 for their analytical expression). The state at the end of the stroke (II $\rightarrow$ III) clearly depends on the chosen protocol, and so does the energy cost for connection

$$E_c^{(s)}(\theta) = -\gamma_0\left\{\langle\hat{\sigma}_A^x\rangle + \cos(2\theta)\left[\cos(2\alpha)(\langle\hat{\sigma}_A^x\rangle + \langle\hat{\sigma}_A^x\hat{\sigma}_B^x\rangle) - \langle\hat{\sigma}_A^y\hat{\sigma}_B^y\rangle - \sin(2\alpha)(\langle\hat{\sigma}_A^z\rangle + \langle\hat{\sigma}_A^z\hat{\sigma}_B^z\rangle)\right]\right\}, \quad (3.15)$$

where θ is the arbitrary phase of the unitary operation in Eq. (2.27) acting on the single qubit,

$$E_c^{(l)}(\theta) = -\gamma_0\cos(2\theta)\left(\cos^2(2\alpha)\langle\hat{\sigma}_A^x\hat{\sigma}_B^x\rangle - \langle\hat{\sigma}_A^y\hat{\sigma}_B^y\rangle + \sin^2(2\alpha)\langle\hat{\sigma}_A^z\hat{\sigma}_B^z\rangle - \sin(4\alpha)\langle\hat{\sigma}_A^x\hat{\sigma}_B^z\rangle\right), \quad (3.16)$$

where $\theta \equiv \theta_A + \theta_B$ is the sum of the arbitrary phases θ_k of each local unitary $\hat{U}_k(\theta_k)$ acting on the k -th qubit, and $E_c^{(g)} \equiv 0$. Note that in the l -JQB case, although the local ergotropy is extracted separately from each qubit, there is only one independent effective parameter.

In the following Sections, we investigate the performance of the proposed QB described by the Hamiltonian in Eq. (3.11). In Section 3.3, we discuss the ideal performance of the working cycle of the p -JQB, while in Section 3.4 we simulate the case of the s -JQB on actual IBM superconducting quantum machines.

3.3 Teoretical results

The performance of the three JQBs described above is summarized in Fig. 3.2, where the extracted work $\mathcal{E}^{(p)}$ with corresponding efficiency of the cycle $\eta^{(p)}(\theta)$ is shown varying γ_0 at fixed temperature $T = 0.5\Omega$ (upper panels) or varying T at fixed $\gamma_0 = 0.8$ (lower panels). First, the efficiency of the (s, l) -JQB is maximum for

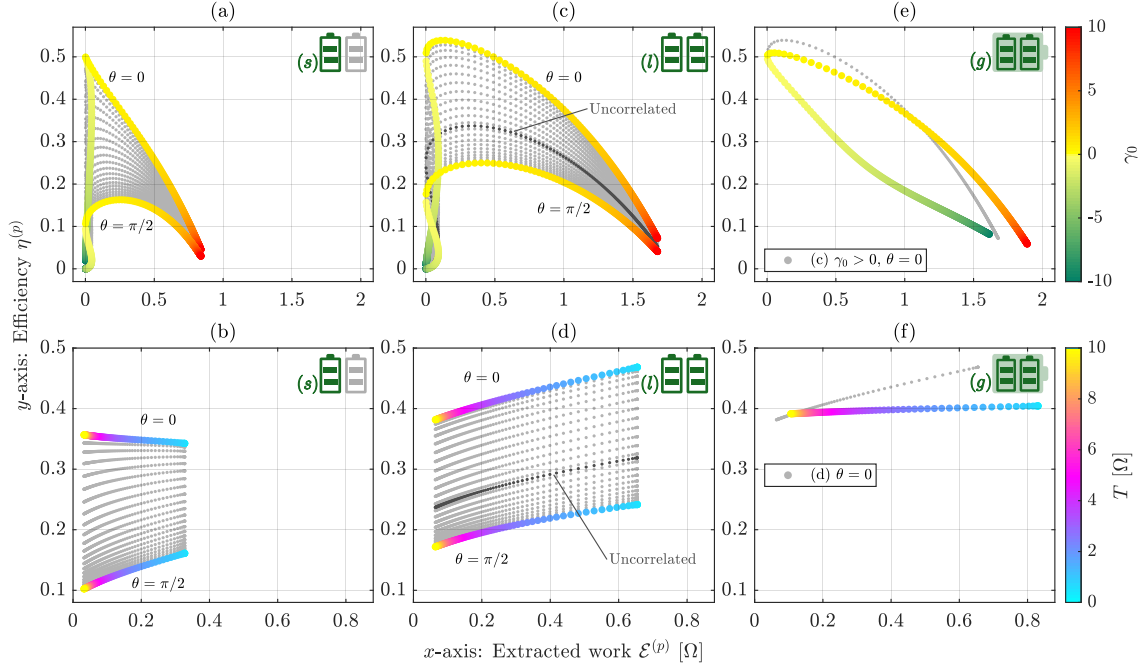


Figure 3.2: Performance of the p -JQB operated under different protocols p in terms of efficiency $\eta^{(p)}$ vs extracted work $\mathcal{E}^{(p)}$: (a,b) s -JQB (single ergotropy, one qubit as a resource); (c,d) l -JQB (local ergotropy, both qubits as a resource); and (e,f) g -JQB (global ergotropy, both qubits and correlations as a resource). (a,c,e) Parametric plot of $\eta^{(p)}$ vs $\mathcal{E}^{(p)}$ for $0 \leq \theta \leq \pi/2$ and $-10 \leq \gamma_0 \leq 10$ at $T = 0.5\Omega$. (b,d,f) Same as in (a,c,e) but for $0 \leq T \leq 10\Omega$ at $\gamma_0 = 0.8$. (a-d) Optimal trade-off between η and $\mathcal{E}$ (Pareto front) is obtained at $\theta = 0$ with $\gamma_0 > 0$. (e,f) Results do not depend on arbitrary phases, since ergotropy is extracted by a global cyclic unitary. In panels (c) and (d), as references, we have reported the results for the case in which disconnection also erases correlations between the two qubits (dark gray dots). In panels (e) and (f), as references, we have reported the best results achieved in panels (c) and (d) respectively (gray dots). For sake of completeness, we have considered values of γ_0 and of T in a range wider than the typical values admissible for the specific superconducting setup discussed in App. C.1. Image taken from [22].

$\theta = 0$, and minimum for $\theta = \pi/2$ [panels (a-d)]. Looking for the optimal trade-off (Pareto front) between $\mathcal{E}^{(p)}$ and $\eta^{(p)}(\theta)$, the conditions (γ_0, θ) under which we cannot further improve one quantity without degrading the other, we conclude that the optimal performance is obtained for $\theta = 0$ with $\gamma_0 > 0$. Second, $\mathcal{E}^{(l)} = 2\mathcal{E}^{(s)} = 2\mathcal{E}$, trivially, but remarkably, the local extraction of ergotropy from both qubits also enhances the efficiency [panels (a-d)]. Third, the most striking result is the presence of parameter regions where, at parity of extracted work, the l -JQB is more efficient than the g -JQB [panels (c-f)]. A few remarks are in order to clarify this point. The protocols considered in this working cycle, the unitaries in the stroke (II $\rightarrow$ III), aim at maximizing the work extractable by cyclic unitary processes (ergotropy), not the efficiency of the cycle. Then, a constrained optimization of the efficiency is performed with respect to the arbitrary phases of the unitary, if any. The constraint is that the unitary must extract ergotropy and, for the g -JQB, phases are irrelevant. When the optimization target is the ergotropy, which is the present case, clearly $\mathcal{E}^{(g)} \geq \mathcal{E}^{(l)}$. Limited to the regime in which both the l - and the g -JQB extract the same amount of work, there exist a set of parameters under which $\eta^{(l)} > \eta^{(g)}$.

There is another point to stress in order to get an intuitive reason of why, provided the same extracted work, the efficiency of the l -JQB can exceed that of the g -JQB.² One could naively expect $\eta^{(g)} \geq \eta^{(l)}(\theta)$, because of $E_c^{(g)} = 0$. However, the fact is that $E_c^{(l)}(\theta)$ is not necessarily an energy cost, positive, because, as shown in Eq. (3.16), the magnitude and sign of the latter depend on θ as $E_c^{(l)}(\theta) \propto \cos(2\theta)$. Whenever the chosen parameter regions for the l - and g -JQB allow for the same ergotropy extraction and the total energy cost for disconnection/connection in the l -JQB is lower than the energy cost of disconnection in the g -JQB, we observe that $\eta^{(l)} > \eta^{(g)}$ [panel (e) of Fig. 3.2] – see also Eq. (3.4).

Concerning the role of temperature at given $\gamma_0 = 0.8$ [Fig. 3.2(b,d,f)], we observe that the lower the temperature, the higher the extracted work. The dependence of the efficiency on the T is weak or even negligible in the s - and in the g -JQB, respectively, while it is more pronounced in the l -JQB. For the l -JQB, higher (lower) values of ergotropy and efficiency are attained at lower (higher) T .

Focusing on the l -JQB, we can consider the case in which the instantaneous disconnection also erases the correlations between the qubits, i.e., $\varrho_{\text{II}} = \rho_A \otimes \rho_B$ with $\rho_A = \text{Tr}_B[\tau_\beta] = \rho_B$ (because of the symmetry of τ_β). The energy cost of disconnection $E_d = \text{Tr}[(\hat{\mathcal{H}}_A + \hat{\mathcal{H}}_B)\rho_A \otimes \rho_B] - \text{Tr}[\hat{\mathcal{H}}\tau_\beta]$ turns out to be equal to Eq. (3.13). By construction, the ergotropy is the same as $\mathcal{E}^{(l)}$. After ergotropy extraction, the system is in the state $\varrho_{\text{III}} = \frac{1}{4}(1 - r\hat{\sigma}_A^z) \otimes (1 - r\hat{\sigma}_B^z)$, which is diagonal in the computational basis, see Eq. (1.2), and so the energy cost of connection is zero (the proof is analogous to that of $E_c^{(g)}$ in App. C.2.2). Therefore, the efficiency of this cycle reads $\eta_{\text{uncorr}}^{(l)} = \mathcal{E}^{(l)}/E_d = \eta^{(l)}(\pi/4)$, since $E_c^{(l)}(\pi/4) = 0$, see Eq. (3.16). This result highlights the relevance of phase coherence in the presence of correlations in our model. Indeed, as shown in Fig. 3.2(c,d), with a suitable choice of the angle θ the performance of the correlated l -JQB can be consistently improved with respect to the uncorrelated case. The latter, instead, cannot benefit from phase-coherence because once correlations are erased, the state after ergotropy extraction is independent of

²Note that, in general, at a given temperature the l -JQB provides the same ergotropy as that of the g -JQB for different values of γ_0 , which, in turn, also results in different values of E_d in Eq. (3.13).

the phases introduced by the unitary operation in Eq. (2.17).

3.4 Simulation on superconducting quantum computers

After theoretically investigating the performance of the JQB in ideal conditions, we have simulated its functioning on a quantum computer. In order to do so, we have used the quantum simulator `aer_simulator`³, without noise on the gates, and the quantum machines `ibm_cairo`⁴ (with restrained access), which is one of the IBM Quantum Falcon processors with 27 qubits, and `ibm_brisbane`⁵ (with open access), which is one of the IBM Quantum Eagle processors with 127 qubits. All these platforms are accessible via the Qiskit package [157]. As we have already mentioned in Section 2.3, these platforms are based on superconducting qubits, however they differ from the one we propose in App. C.1 for our cyclic QB. Therefore, it is worth commenting preliminarily about the different setups and outlining how the simulation is carried out. The minimal model for a cyclic QB in App. C.1 is based on dc-SQUID charge qubits, designed to operate in the regime $E_J \ll E_C$. As already mention in Section 1.2.3, these charge qubits, however, are not suited for quantum computing, because environmental charge noise strongly limits their coherence times [158]. For this reason IBM quantum hardwares are currently based on transmons [77].

Unless one has access to low-level controls on the hardware, the operations one can perform on a quantum computer are limited to unitaries and measurements. Considering this constraint and the different setup of IBM quantum processors with respect to ours, simulating the proposed thermodynamic cycle does not consist in rigorously performing each stroke, e.g, connection and disconnection, but rather in preparing the two-qubit states required to assess the energetics of the cycle. The simulation is thus carried out as a two-step process: (i) The initial Gibbs state is prepared in the quantum register and a quantum state tomography (QST) is performed; (ii) The initial Gibbs state is prepared again from scratch, it undergoes the unitary work extraction, and then a QST is performed. The QSTs are required to reconstruct the states that are actually implemented in the quantum register before and after work extraction. Such states, in turn, allow us to determine the proper unitary for work extraction and the energetics of the cycle, upon computing the expectation values of the Hamiltonian after each stroke as per Section 3.3.

In this framework, the parameters characterizing the QB, i.e., the temperature T and the coupling strength γ_0 , are thus implicitly encoded in the preparation of the initial Gibbs state.

3.4.1 Generation of the initial Gibbs state

The first, and most critical, step needed to simulate a thermodynamic cycle like the one discussed above, is the preparation of the initial Gibbs state τ_β . Indeed,

³The `aer_simulator` is a classical high-performance simulator provided within Qiskit, allowing one to emulate ideal quantum circuits without hardware noise.

⁴This device has been officially retired by IBM on April 30th, 2024.

⁵This device has been officially retired by IBM on November 3rd, 2025.

quantum computers are specifically designed to perform reversible unitary quantum operations and measurements [69]. Therefore, it is not straightforward for an end user to realize mixed states using them. A possible way to overcome this issue is to rely on the so called thermofield double (TFD) states [159–162]. The idea behind this approach is to generate a pure state (the TFD state) in an enlarged system made up of two identical copies of the quantum system under investigation in such a way that tracing out the degrees of freedom of one of the two copies the other is described by the desired Gibbs state. In the following, we will use the notation introduced above for the system under investigation S and we will add a prime index to distinguish the ancillary system S' .

To proceed further in this direction, we consider the Hamiltonian $\hat{\mathcal{H}}$ in Eq. (3.11), defined in the Hilbert space of the system S , and a formally identical Hamiltonian $\hat{\mathcal{H}}'$ defined in the Hilbert space of the ancillary system S' . The TFD state is then defined on the enlarged Hilbert space and can be written as

$$|\text{TFD}(\beta)\rangle = \sum_{k=1}^d \frac{e^{-\frac{\beta \varepsilon_k}{2}}}{\sqrt{\text{Tr}[e^{-\beta \hat{\mathcal{H}}}]}} |\epsilon_k\rangle_S |\epsilon'_k\rangle_{S'}. \quad (3.17)$$

As can be expected, by tracing out the degrees of freedom of the ancillary system S' , one recovers the Gibbs state τ_β for the system S introduced in Eq. (2.29). Moreover, in the specific case under investigation we have $d = 4$.

To realize the state in Eq. (3.17) we first apply two Hadamard gates (H) and two CNOT gates (blue region in the scheme of Fig. 3.3) to initialize the enlarged system in the state

$$|\text{TFD}(0)\rangle = \frac{1}{2} (|0\rangle_A |0\rangle_{A'} + |1\rangle_A |1\rangle_{A'}) \otimes (|0\rangle_B |0\rangle_{B'} + |1\rangle_B |1\rangle_{B'}). \quad (3.18)$$

We then use a variational scheme with an ansatz motivated by quantum-approximate

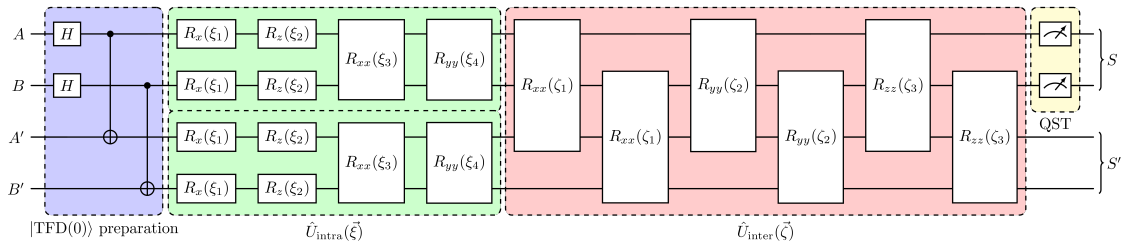


Figure 3.3: Quantum circuit associated to a single-step of the protocol that determines the optimal parameters to initialize the system S in the Gibbs state. Blue area: preparation of the state $|\text{TFD}(0)\rangle$ in Eq. (3.18); green area: unitary operation acting separately on the system S and S' ; red area: unitary operation coupling the system S and S' ; yellow area: QST to determine the state of the system S . Here, we have used the gates $R_i^J(\theta) = e^{-i\frac{\theta}{2}\hat{\sigma}_J^i}$ and $R_{ii}^{JK}(\theta) = e^{-i\frac{\theta}{2}(\hat{\sigma}_J^i \otimes \hat{\sigma}_K^i)}$ with $i = x, y, z$ and $J, K = A, A', B, B'$ to implement the unitaries introduced in the main text. Image taken from [22].

optimization algorithms [163] where intra-system and inter-system unitary operations are alternated. The former class of unitaries (green region in Fig. 3.3) acts

separately to S and S' and can be written as

$$\begin{aligned}\hat{U}_{\text{intra}}(\vec{\xi}) &= e^{-i\frac{\xi_4}{2}(\hat{\sigma}_A^y \otimes \hat{\sigma}_B^y + \hat{\sigma}_{A'}^y \otimes \hat{\sigma}_{B'}^y)} \\ &\times e^{-i\frac{\xi_3}{2}(\hat{\sigma}_A^x \otimes \hat{\sigma}_B^x + \hat{\sigma}_{A'}^x \otimes \hat{\sigma}_{B'}^x)} \\ &\times e^{-i\frac{\xi_2}{2}(\hat{\sigma}_A^z + \hat{\sigma}_B^z + \hat{\sigma}_{A'}^z + \hat{\sigma}_{B'}^z)} \\ &\times e^{-i\frac{\xi_1}{2}(\hat{\sigma}_A^x + \hat{\sigma}_B^x + \hat{\sigma}_{A'}^x + \hat{\sigma}_{B'}^x)},\end{aligned}\quad (3.19)$$

while the latter (red region in Fig. 3.3) couples S and S' and reads

$$\begin{aligned}\hat{U}_{\text{inter}}(\vec{\zeta}) &= e^{-i\frac{\zeta_3}{2}(\hat{\sigma}_A^z \otimes \hat{\sigma}_{A'}^z + \hat{\sigma}_B^z \otimes \hat{\sigma}_{B'}^z)} \\ &\times e^{-i\frac{\zeta_2}{2}(\hat{\sigma}_A^y \otimes \hat{\sigma}_{A'}^y + \hat{\sigma}_B^y \otimes \hat{\sigma}_{B'}^y)} \\ &\times e^{-i\frac{\zeta_1}{2}(\hat{\sigma}_A^x \otimes \hat{\sigma}_{A'}^x + \hat{\sigma}_B^x \otimes \hat{\sigma}_{B'}^x)}.\end{aligned}\quad (3.20)$$

Notice that the form of Eq. (3.19) is motivated by the single- and two-qubit terms appearing in the Hamiltonian in Eq. (3.11), while Eq. (3.20) is built extending the same idea to include coupling among the S and S' [160, 161].

Altogether they lead to the unitary

$$\hat{U}_{\text{TFD}}(\vec{\xi}, \vec{\zeta}) = \hat{U}_{\text{inter}}(\vec{\zeta}) \hat{U}_{\text{intra}}(\vec{\xi}), \quad (3.21)$$

where the variational parameters $\vec{\xi} = (\xi_1, \xi_2, \xi_3, \xi_4)$ and $\vec{\zeta} = (\zeta_1, \zeta_2, \zeta_3)$ need to be optimized to generate the closest state to the target state $|\text{TFD}(\beta)\rangle$ according to a given cost function. The variational parameters implicitly encode the temperature T and the coupling strength γ_0 of the QB. In the present case, we have chosen as cost function the infidelity with respect to the target Gibbs state defined as $1 - F(\tilde{\tau}(\vec{\xi}, \vec{\zeta}), \tau_\beta)$ with

$$\tilde{\tau}(\vec{\xi}, \vec{\zeta}) = \text{Tr}_{S'}[\hat{U}_{\text{TFD}}(\vec{\xi}, \vec{\zeta}) |\text{TFD}(0)\rangle \langle \text{TFD}(0)| \hat{U}_{\text{TFD}}^\dagger(\vec{\xi}, \vec{\zeta})] \quad (3.22)$$

and where

$$F(\rho, \sigma) = \text{Tr} \left[\sqrt{\sqrt{\rho} \sigma \sqrt{\rho}} \right] \quad (3.23)$$

is the conventional definition of the fidelity for two arbitrary density matrices ρ and σ [66]. For completeness, we have also tested other cost functions such as the free energy and weighted sums of the infidelity with various normalized energy components (not shown). However, the latter approaches were not as good in estimating the extracted work and the efficiency of the considered system as the approach based only on the infidelity.

To evaluate the fidelity, we perform a QST (yellow region in the scheme of Fig. 3.3) [66]. This is an experimental procedure that allows to reconstruct the density matrix of a quantum state. It consists in preparing the system in the same state many times and measuring it in a tomographically complete basis of measurement operators. That is, the measured operators must form an operator basis on the Hilbert space of the system.

To obtain the best estimation of the variational parameters $\vec{\xi}$ and $\vec{\zeta}$, the steps discussed above and illustrated in Fig. 3.3 were implemented using the simulator without noise with number of shots equal to 1000. After every QST the optimization of the parameters was performed via a Bayesian optimisation [164, 165], an approach

which is particularly convenient when the cost function to optimize is a black box for which no closed form is known (nor its gradients), is computationally expensive to evaluate and noisy. These conditions perfectly fit the case under investigation. The achieved parameters were then fed back into the quantum circuit of Fig. 3.3 starting another round of optimization. This procedure was iterated for a number of times sufficient to reach a convergence of the results for the density matrix of S (typically 400-600). In Fig. 3.4 we report a scheme of the whole optimization algorithm.

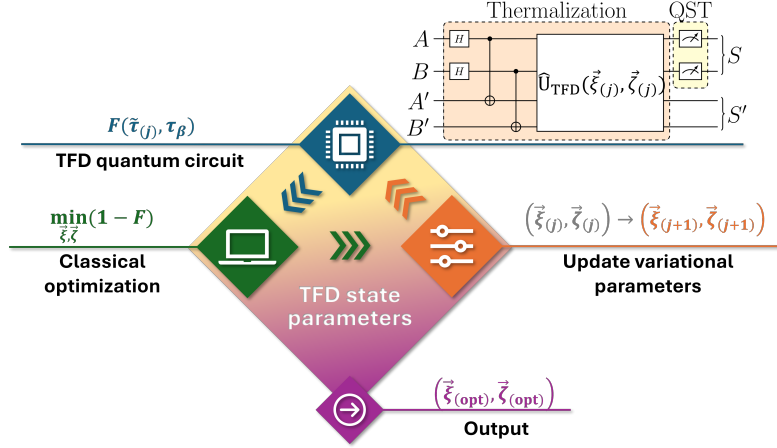


Figure 3.4: Scheme of the variational algorithm used to prepare the TFD state. In each iteration (j) the quantum circuit in Fig. 3.3 is executed to determine the fidelity F between the state $\tilde{\tau}_{(j)} \equiv \tilde{\tau}(\vec{\xi}_{(j)}, \vec{\zeta}_{(j)})$ and the target Gibbs state, τ_β (blue part). The infidelity ($1 - F$) is then minimized via a Bayesian optimization, performed on a classical computer (green part), in order to update the circuit parameters in $(\vec{\xi}_{(j+1)}, \vec{\zeta}_{(j+1)})$ (orange part) and start a new iteration, ($j + 1$). This procedure is iterated until the algorithm converges, yielding the optimal parameters $(\vec{\xi}_{(opt)}, \vec{\zeta}_{(opt)})$ (violet part). Image taken from [22].

3.4.2 Simulation of the thermodynamic cycle

Once the parameters leading to the best approximation of the thermal state for S were obtained, we moved on to the simulation of the whole thermodynamic cycle, both using the simulator and the two real devices mentioned above. One purpose of this simulation is to perform a feasibility test of the protocols based on the extraction of local ergotropies. Since the principle is equivalent for both the s - and the l -JQB, ergotropy is locally extracted from each qubit by single-qubit gates, which can be eventually executed in parallel, without loss of generality we restrict the discussion to the s -JQB. Note that during strokes (I $\rightarrow$ II) and (III $\rightarrow$ IV) the density matrix of the bipartite system does not change. This means that we do not have to perform any operation on the qubits to simulate these strokes.

Here, the extraction of ergotropy from the single qubit is straightforwardly implemented on the quantum computer as the product of two single-qubit rotation gates, see Eq. (2.27). For the simulation, we consider the regime where the best performance is ideally expected, i.e., $\gamma_0 > 0$ with $\theta = 0$ (Fig. 3.2(a,b)). The latter assumption further simplifies the unitary in Eq. (2.27) to a single-qubit rotation

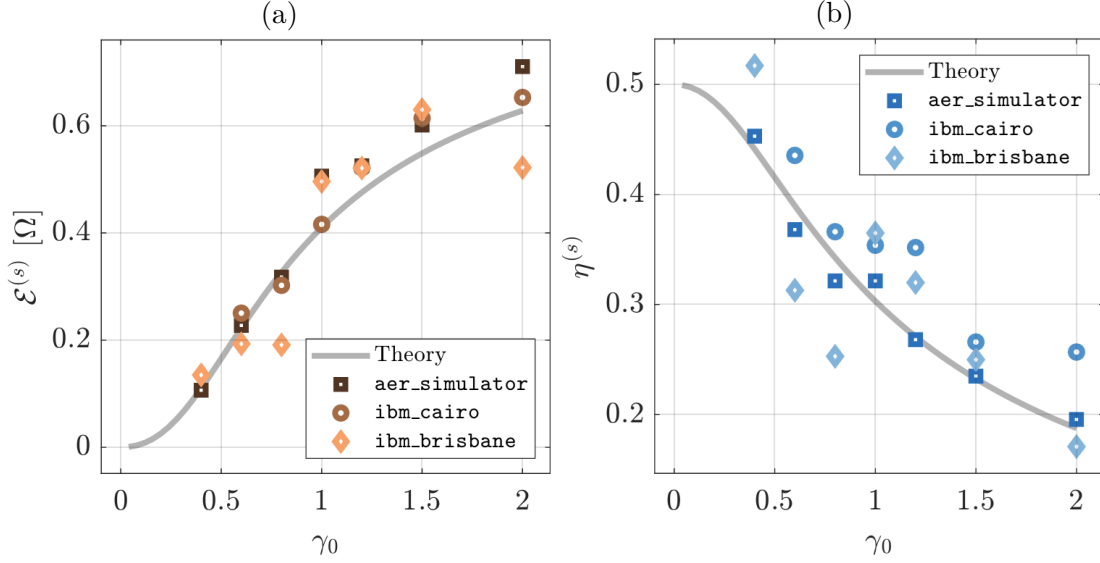


Figure 3.5: Performance of the simulated s -JQB at $T = 0.5\Omega$ and $\theta = 0$. (a) Extracted work $\mathcal{E}^{(s)} = \mathcal{E}$ and (b) efficiency $\eta^{(s)}$ as a function of $0 < \gamma_0 \leq 2$ for the ideal cycle starting with a Gibbs state (gray curve) and for the cycles starting with a thermal double state (markers) simulated on (`aer_simulator`) and actual quantum hardware (`ibm_cairo` and `ibm_brisbane`). Image taken from [22].

about the y -axis. In this regard, the parameter α in Eq. (2.27) was directly evaluated from the coordinates on the Bloch sphere of the density matrix achieved after the thermalization. Fig. 3.5 shows the performance of the simulated s -JQB in terms of the extracted work $\mathcal{E}^{(s)}$ [panel (a)] and of the efficiency $\eta^{(s)}$ [panel (b)] at a given temperature ($T = 0.5\Omega$) and for different values of the coupling $\gamma_0 \in [0.4, 2]$. We focused our analysis on this region of parameters to achieve a good signal-to-noise ratio, as indicated by the ideal results shown in Fig. 3.2(a,b). For $\gamma_0 < 0.4$, we expect very small values of ergotropy, whereas for $\gamma_0 > 2$, we expect low cycle efficiencies, making the measurement of these quantities more challenging. Moreover, for $T > \Omega$, we observed issues with the convergence of the variational algorithm when preparing the initial Gibbs state. Conversely, for $T < \Omega$ we do not expect a strong dependence of the ergotropy and the efficiency on T , therefore, we have fixed $T = 0.5\Omega$. Despite these limitations in the choice of viable parameters for the simulation, we point out that those we considered are consistent with the experimentally admissible configuration of the dc-SQUID setup discussed at the end of App. C.1. The simulator data were generated by using 1000 shots and averaging over 30 runs. In contrast, the data from the real machine were obtained from a single run with 4000 shots. Note that reproducing the circuit in Fig. 3.3 requires 4 qubits with a square connection, which is not available in the devices we have used. To minimize the necessary SWAP gates, we utilized 4 qubits connected in a linear configuration (the mapping of qubits $[A, B, A', B']$ is $[18, 24, 21, 23]$ for `ibm_cairo` and $[32, 17, 31, 30]$ for `ibm_brisbane`, see Fig. 3.6).

For both the ergotropy and the efficiency the agreement between the data obtained from the simulator and the two considered real quantum devices and the theoretical curves is good. We observe, however, that the agreement for the ergo-



Figure 3.6: Qubit connectivity map of (a) `ibm_cairo` and (b) `ibm_brisbane`, with the qubits used for the simulations highlighted in orange and blue, respectively. Image taken from [22].

trophy [panel (a)] is better than that for efficiency [panel (b)]. The reason of this can be traced back to the definitions of the considered quantities. Indeed, after performing the QST to obtain the density matrix of the system S before and after the ergotropy extraction, accomplished by applying the rotation in Eq. (2.27), the extracted work $\mathcal{E}^{(s)}$ is numerically evaluated in a unique step. Instead, assessing the efficiency $\eta^{(s)}$ requires multiple steps. First, it requires the separate calculation of $\mathcal{E}^{(s)}$, $E_c^{(s)}$, and E_d . These quantities are then combined to construct $\eta^{(s)}$ as in Eq. (3.4). When performing calculations with quantities affected by errors, these errors propagate through each step, consequently, the individual errors from $\mathcal{E}^{(s)}$, $E_c^{(s)}$, and E_d combine and potentially accumulate, leading to a greater overall error in the final calculation of $\eta^{(s)}$.

In this regard, errors have different possible origins. One source of error is associated to the parameter optimization required to simulate the initial Gibbs state τ_β . In the cases shown here, the fidelity between the ideal Gibbs state and the one obtained following the optimization procedure ranges between 0.95 and 0.98. This error affects all data at a given γ_0 in the same way, since the parameter optimization is performed once for each value of γ_0 using the `aer_simulator`. The other main sources of error are: (i) the intrinsic noise of the quantum computers (gates, readout, and qubit decoherence) and (ii) the probabilistic nature of the measurements, performed in a finite number. For the considered IBM quantum devices the qubit state stability is of the order of $100 \mu\text{s}$, the gates acting on the qubits have median single-qubit gate error $\sim 10^{-4}$, while the median two-qubit gate error and the median readout error are $\sim 10^{-2}$ [157]. As regard the probabilistic nature of the measurements we recall that we have performed 1000 shots repeated for 30 runs on the simulator and 4000 shots for a single run on the real devices.

As it clearly emerges from this brief description, the sources of error affecting the simulation are numerous and of various nature. For this reason, estimating the error affecting the data reported in Fig. 3.5 starting from these sources is very challenging. We can, however, estimate the magnitude of such errors starting from another observation. As already mentioned, the fidelity between the ideal Gibbs state and the one obtained on the simulator ranges from 0.95 to 0.98 (average 0.97). Similarly, we have that the fidelity between the ideal Gibbs state and the one obtained on real machines ranges from 0.85 to 0.97 (average 0.91). In the first case, the deviation from 1 of the fidelity is attributed to the error in determining the parameters to construct the initial state, while in the second case all the errors described above combine. At this point, it seems reasonable to assume the parameter $1 - F$, with

F the fidelity, as the relative error on each QST, thus on the determination of each density matrix. This will therefore be of the order of 3% for the simulators and of 10% for the real devices. Note that the argumentation has been made on the state before the extraction of ergotropy, but it is legitimate to extend it also to the state after the extraction of ergotropy since the difference associated to the $\hat{\sigma}_y$ rotation (corresponding to 4 native single-qubit gates) on the entire process can be safely neglected. Propagating the errors through the usual rules, we can estimate a relative error of about 20% for the ergotropy and of about 40% for the efficiency. This estimation appears reasonable when compared with the obtained results (see Fig. 3.5).

Chapter 4

Dynamical blockade of a reservoir for optimal performances of a quantum battery

The goal of this Chapter is to demonstrate that it is possible to design a fast and efficient QB based on a harmonic oscillator strongly coupled to a highly non-Markovian thermal reservoir, characterized by a cut-off frequency $\omega_D \gtrsim \omega_0$ and dissipation $\gamma_0 \gg \omega_0$, with ω_0 frequency of the oscillator. In such a regime, at short enough times, the switch-on coupling energy between QB and reservoir is almost completely transferred directly to the QB itself with only marginal dissipation onto the reservoir degrees of freedom, due to a *dynamical blockade* of the reservoir [166]. We explain this dynamical blockade in terms of the hybridization between the QB and the reservoir modes with frequency close to a new emergent frequency $\Omega = \sqrt{\gamma_0 \omega_D} \gg \omega_0$ ¹. We point out that, in this underdamped regime, almost all the energy accumulated in the QB can be extracted. In addition, for short enough times the energy oscillates back and forth in an almost periodic and coherent way between the coupling energy and the QB, and the robustness of this effect over various periods of these energy oscillations can be exploited to mitigate the need for precise fine-tuning of the charging time. Furthermore, our results are robust up to the thermal energies comparable with Ω .

The results of this work have been published in Ref. [36], and this Chapter is largely based upon it.

4.1 Model of the QB and reservoir

The Hamiltonian of the system consists of three terms

$$\hat{\mathcal{H}}(t) = \hat{\mathcal{H}}_B + \hat{\mathcal{H}}_R + \hat{\mathcal{H}}_{\text{int}}(t). \quad (4.1)$$

The QB is a quantum harmonic oscillator which is described by the Hamiltonian in Eq. (2.33). It is strongly coupled to a many-modes reservoir described as a large collection of quantum harmonic oscillators in the framework of the Caldeira-Leggett

¹Note that the frequency Ω will be used as reference scale in the plots of this Chapter, as in the previous one. This is why we use the same symbol, even though it has two different physical origins in the two Chapters.

model [63, 64, 167, 168] whose Hamiltonian reads

$$\hat{\mathcal{H}}_{\text{R}} = \sum_k \hat{\mathcal{H}}_{\text{R}}^{(k)} = \sum_k \left(\frac{\hat{p}_k^2}{2m_k} + \frac{m_k \omega_k^2}{2} \hat{x}_k^2 \right), \quad (4.2)$$

where $\hat{x}_k$ and $\hat{p}_k$ are the position and momentum of the k -th mode, with mass m_k and characteristic frequencies ω_k . The QB and the reservoir are coupled through the term

$$\hat{\mathcal{H}}_{\text{int}}(t) = \theta(t) \hat{\mathcal{H}}_{\text{int}} \quad (4.3)$$

with

$$\hat{\mathcal{H}}_{\text{int}} = \sum_k \hat{\mathcal{H}}_{\text{int}}^{(k)} = - \left(\sum_k c_k \hat{x}_k \right) \hat{x} + \frac{1}{2} m \Omega^2 \hat{x}^2 \quad (4.4)$$

which, as will be shown, plays the role of a quantum charger. Eq. (4.4) is composed of two terms: a bilinear coupling between $\hat{x}$ and $\hat{x}_k$, with c_k coupling constants which will be specified later on, and a counter-term proportional to $\hat{x}^2$, where

$$\Omega^2 = \sum_k \frac{c_k^2}{m m_k \omega_k^2}. \quad (4.5)$$

Since Ω vanishes for $c_k \rightarrow 0$, the counter-term is itself a part of the coupling Hamiltonian even though it only depends on the QB coordinate from the theoretical point of view. It is needed to prevent the renormalization of the static potential of the QB pinning its frequency to the bare value ω_0 [63, 64]. Its presence depends on the specific considered model, in particular it naturally emerges in the description of solid-state platforms based on superconducting circuits [169], as will be discussed in more details in the App. D.1, devoted to the experimental feasibility. Moreover, it plays a relevant role in the context of energy storage and extraction, as will be clear in the following.

The equations of motion for the QB and reservoir position operators in the Heisenberg picture read

$$\ddot{\hat{x}}(t) + (\omega_0^2 + \Omega^2) \hat{x}(t) = \sum_k \frac{c_k}{m} \hat{x}_k(t), \quad (4.6)$$

$$\ddot{\hat{x}}_k(t) + \omega_k^2 \hat{x}_k(t) = \frac{c_k}{m_k} \hat{x}(t). \quad (4.7)$$

Eq. (4.7) can be formally solved considering $\hat{x}(t)$ a given external field, yielding

$$\hat{x}_k(t) = \hat{x}_k(0) \cos(\omega_k t) + \frac{\hat{p}_k(0)}{m_k \omega_k} \sin(\omega_k t) + \frac{c_k}{m_k \omega_k} \int_0^t dt' \sin[\omega_k(t-t')] \hat{x}(t'). \quad (4.8)$$

Replacing this solution into Eq. (4.6) we obtain the full operatorial quantum Langevin equation for the QB [64, 170–172]

$$\ddot{\hat{x}}(t) + \omega_0^2 \hat{x}(t) + \int_0^t dt' \gamma(t-t') \dot{\hat{x}}(t') + \gamma(t) \hat{x}(0) = \frac{\hat{\xi}(t)}{m}, \quad (4.9)$$

where the damping kernel

$$\gamma(t) = \frac{1}{m} \theta(t) \sum_k \frac{c_k^2}{m_k \omega_k^2} \cos(\omega_k t) \quad (4.10)$$

and the reservoir fluctuating noise operator

$$\hat{\xi}(t) = \sum_k c_k \left[\hat{x}_k(0) \cos(\omega_k t) + \frac{\hat{p}_k(0)}{m_k \omega_k} \sin(\omega_k t) \right] \quad (4.11)$$

have been introduced.

The solution of Eq. (4.9) can always be decomposed into a transient homogeneous (h) and a non-homogeneous or thermal part (th):

$$\hat{x}(t) = \hat{x}_h(t) + \hat{x}_{th}(t). \quad (4.12)$$

The first term is independent of the fluctuating field $\hat{\xi}(t)$ and is expressed via the response function $\chi(t)$ in terms of the initial conditions at time $t = 0$ as

$$\hat{x}_h(t) = \hat{x}(0)\chi(t) + \hat{x}(0)\dot{\chi}(t). \quad (4.13)$$

All the properties of $\chi(t)$, which satisfies initial conditions $\chi(0) = 0$, $\dot{\chi}(0) = 1$ and $\ddot{\chi}(0) = 0$, are encoded into its Laplace transform (defined as $\hat{\chi}(\lambda) = \int_0^{+\infty} dt e^{-\lambda t} \hat{x}(t)$)

$$\tilde{\chi}(\lambda) = \frac{1}{\lambda^2 + \omega_0^2 + \lambda \tilde{\gamma}(\lambda)}, \quad (4.14)$$

where $\tilde{\gamma}(\lambda)$ is the Laplace transform of Eq. (4.10).

The term $\hat{x}_{th}(t)$ in Eq. (4.12) depends instead on the fluctuating field $\hat{\xi}(t)$ and is given by

$$\hat{x}_{th}(t) = \int_0^t \frac{dt'}{m} \chi(t-t') \hat{\xi}(t'). \quad (4.15)$$

4.2 The charging/discharging protocol

The charging/discharging protocol is comprised of four steps:

- (I) *Connection.* At $t = 0$, switching on $\hat{\mathcal{H}}_{\text{int}}(t)$ the QB and the reservoir are connected;
- (II) *Charging.* Energy flows for a short amount of time t ;
- (III) *Disconnection.* Switching off $\hat{\mathcal{H}}_{\text{int}}(t)$, the QB and the reservoir are disconnected;
- (IV) *Ergotropy extraction.* The maximum amount of energy can be extracted from the QB, to be employed elsewhere. In steps (I) and (III) the switching on and off times are assumed as the shortest time scales involved in the problem.

A suitably engineered reservoir, especially within the protocol described above, will prove to be a valuable resource allowing fast and optimal charging of the QB.

4.2.1 Performances of the charging/discharging protocol

In order to assess the performances of the charging procedure, in this framework two different efficiencies can be considered. The first is

$$\eta_B(t) = \frac{\mathcal{E}(t)}{\langle H_B(t) \rangle} = 1 - \frac{\omega_0 \sqrt{\det \sigma_B(t)}}{\langle H_B(t) \rangle}, \quad (4.16)$$

namely the ratio between the ergotropy and the energy stored in the QB, following the definitions given respectively in Sections 2.2.3 and 2.2.1. The second figure of merit is

$$\eta_W(t) = \frac{\mathcal{E}(t)}{W(t)} \quad (4.17)$$

representing the ratio between the maximum work that can be extracted from the QB and the work paid to switch on and off the charger, following the definitions given respectively in Sections 2.2.3 and 2.2.4.

In accordance with the discussion in Section 2.2.4, $\eta_W(t)$ is expected to reach its optimal values under very rapid switching of the coupling, while slower protocols may result in reduced performance. This definition aligns with standard practice in the quantum battery literature, where the energy cost of engineering the bath is typically neglected [149]. This simplification is justified by modeling the bath, within the Caldeira-Leggett framework used here, as a collection of passive elements, such as capacitances and inductances [169], maintained at a fixed temperature and thermalized prior to the charging protocol. However, unlike the previous Chapter, we are not considering a thermodynamic cycle. As a result, a proper definition of the efficiency in Eq. (4.17) should include the entropy production term in the denominator. Nevertheless, within the parameter range considered, this contribution is typically very small. Therefore, we will safely neglect it in the following analysis.

Using the Langevin equation in Eq. (4.6), $\langle \hat{\mathcal{H}}_{\text{int}}(t) \rangle$, that is necessary to evaluate the work, can be expressed in terms of the QB variables as

$$\frac{\langle \hat{\mathcal{H}}_{\text{int}}(t) \rangle}{m} = \langle \hat{x}^2(t) \rangle - \frac{1}{2} \frac{d^2}{dt^2} \langle \hat{x}^2(t) \rangle - \left(\omega_0^2 + \frac{\Omega^2}{2} \right) \langle \hat{x}^2(t) \rangle. \quad (4.18)$$

It is worth noting that this contribution explicitly depends on the counter-term in Eq. (4.4).

4.2.2 Energy balance and spectral decomposition

Since the total system is closed, after the switching on, we can recall the total energy balance in Eq. (2.40), with a clear meaning: the total work $W(t)$ is distributed among the accumulated energy of the battery $\Delta E_B(t)$ and the energy exchanged with the reservoir during the time t . Eq. (2.40) further underlines the role of $\mathcal{H}_{\text{int}}$ as a quantum charger. In this respect, an efficient charging protocol predominantly exchanges energy between the charger and the QB, see Fig. 4.1(a), while an inefficient protocol wastes most of its energy in the reservoir with little power delivered to the QB, as shown Fig. 4.1(b). Even though achieving an efficient charging seems almost hopeless in this context, given that the reservoir has a very large number of degrees of freedom which can collect energy with respect to the single one of the QB,

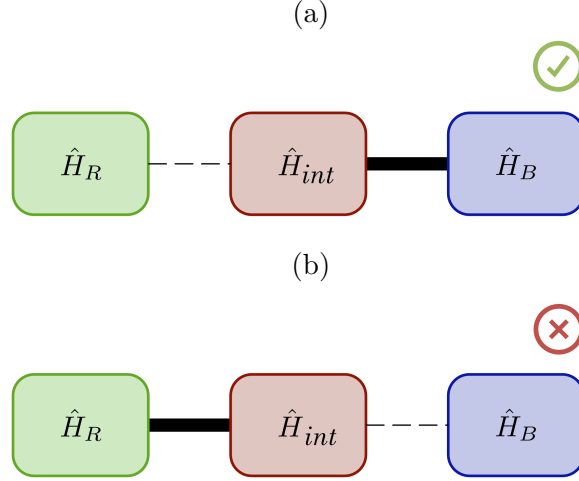


Figure 4.1: Green boxes, reservoir with Hamiltonian $\hat{\mathcal{H}}_R$ defined in Eq. (4.2). Red boxes, charger with Hamiltonian $\hat{\mathcal{H}}_{int}$ defined in Eq. (4.4). Blue boxes, QB with Hamiltonian $\hat{\mathcal{H}}_B$ defined in Eq. (2.33). Panel (a) shows an efficient charging protocol where the energy is predominantly exchanged between the charger and the QB and panel (b) shows an inefficient charging protocol where the energy is predominantly exchanged between the charger and the reservoir. In both panels, the solid thick lines connect the two parts of the system where the dominant energy exchange occurs, while the dashed lines connect the parts where this energy exchange is small. Image taken from [36] with minor modifications.

we will show that this is indeed possible via a careful engineering of the reservoir spectral density at strong coupling.

For later convenience we also introduce the contributions to the interaction Hamiltonian and to the reservoir energy due to the k -th mode of the latter, defined, in complete analogy with Section 2.2.1, as ($\nu = \text{int}, R$)

$$\Delta E_\nu(t, \omega_k) = \langle \hat{\mathcal{H}}_\nu^{(k)}(t) \rangle - \langle \hat{\mathcal{H}}_\nu^{(k)}(0) \rangle \quad (4.19)$$

which satisfy the sum rules

$$\Delta E_\nu(t) = \sum_k \Delta E_\nu(t, \omega_k). \quad (4.20)$$

4.3 Engineered reservoir and operating regimes

4.3.1 The response function

To proceed further with our analysis we need to specify the couplings c_k in the interaction Hamiltonian $\hat{\mathcal{H}}_{int}$. Among the possible choices, we consider the paradigmatic case of Ohmic coupling which is the most common dissipation, especially when the reservoir is represented by quantum circuits [173]. We have [64, 174–176]

$$c_k = \omega_k \sqrt{\frac{2\gamma_0 m m_k \Delta}{\pi} \frac{\omega_D^2}{\omega_D^2 + \omega_k^2}}. \quad (4.21)$$

Here, γ_0 is the coupling strength, ω_D the Drude cut-off, and $\omega_k = k\Delta$ (k positive integer) with Δ the constant level spacing of the modes of the reservoir. The behavior of the couplings defines the spectral density

$$J(\omega) = \frac{\pi}{2} \sum_k \frac{c_k^2}{m_k \omega_k} \delta(\omega - \omega_k), \quad (4.22)$$

and the damping kernel, see Eq. (4.10). Letting the number of modes growing to infinity, while contextually reducing the level spacing ($\Delta \rightarrow 0$), one eventually gets the continuum limit

$$J(\omega) = m\gamma_0\omega \frac{\omega_D^2}{\omega^2 + \omega_D^2} \quad (4.23)$$

$$\gamma(t) = \gamma_0\omega_D e^{-\omega_D t} \theta(t); \quad \tilde{\gamma}(\lambda) = \frac{\gamma_0\omega_D}{\lambda + \omega_D}. \quad (4.24)$$

We can also identify the frequency scale Ω introduced in Eq. (4.5) as

$$\Omega = \sqrt{\gamma_0\omega_D}, \quad (4.25)$$

which, as we will see, will play a crucial role on the charging dynamics of the QB.

As clear from the shape of $\gamma(t)$, the reservoir is highly non-Markovian when ω_D , the inverse of a memory time scale, is small ($\omega_D \approx \omega_0$), a regime of particular interest for this work. Such a regime has in the past drawn theoretical attention [149, 177–179], and has recently been shown to be a resource in quantum thermodynamics [180]. It is also important to stress that such a strong non-Markovian environment can nowadays be experimentally engineered in the context of quantum circuits (see Refs. [181–186] and App. D.1).

We can now explicitly write the Laplace transform of the response function in Eq. (4.14) as [64]

$$\tilde{\chi}(\lambda) = \frac{\lambda + \omega_D}{(\lambda^2 + \omega_0^2)(\lambda + \omega_D) + \lambda\gamma_0\omega_D} \quad (4.26)$$

which, in the time domain, can be written as

$$\chi(t) = \sum_{j=1}^3 \chi_j e^{-\lambda_j t}. \quad (4.27)$$

Here the λ_j are solutions of the equation

$$\lambda^3 - \lambda^2\omega_D + \lambda(\omega_0^2 + \gamma_0\omega_D) - \omega_D\omega_0^2 = 0, \quad (4.28)$$

and

$$\chi_j = (\omega_D - \lambda_j) \prod_{j' \neq j} \frac{1}{\lambda_{j'} - \lambda_j}. \quad (4.29)$$

4.3.2 Operating regimes

As clear from Eq. (4.27), the nature of the roots λ_j , governed by the system parameters, determines the characteristics of $\chi(t)$. From now on, we will elect ω_0 as a typical energy scale and thus consider γ_0 and ω_D as free parameters. As shown in Fig. 4.2, due to the third degree polynomial with real coefficients, only two regimes can occur:

- a *underdamped* (UD) regime (blue part), characterized by one purely real and two complex conjugate roots;
- a *overdamped* (OD) regime (red part), where three real solutions occur.

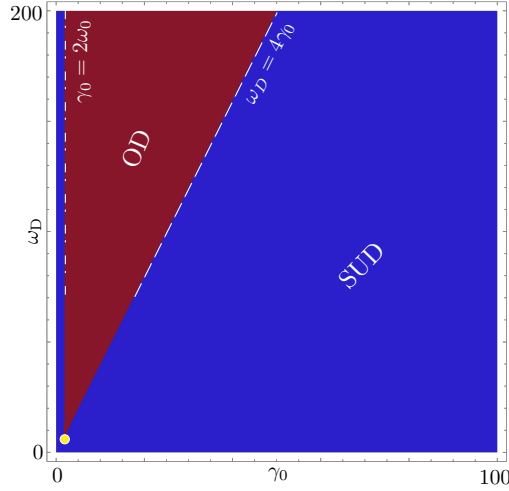


Figure 4.2: As inferred by the nature of the zeroes of Eq. (4.28), as a function of γ_0 and ω_D (units ω_0), the red area denotes the overdamped (OD) regime, while the blue one corresponds to the underdamped (UD) one and, in particular, the strongly underdamped (SUD) in the right part. The bottom corner of the OD regime, marked as a yellow dot, has coordinates $\gamma_0 = \frac{8}{3\sqrt{3}}\omega_0$ and $\omega_D = 3\sqrt{3}\omega_0$. The dash-dotted and dashed lines denote the boundaries between UD and OD for $\omega_D \gg \omega_0$. Image taken from [36].

To enter more into the details let us begin discussing the UD regime, by identifying the two representative regions. The first is the *weakly* UD one, with $\gamma_0 \ll \omega_0, \omega_D$, to the left of the OD part. Here, to leading order in ω_D , $\chi(t)$ exhibits oscillations at the bare frequency ω_0 , damped by the coupling with the reservoir [64, 175]

$$\chi(t) \approx \frac{1}{\omega_0} e^{-\frac{\gamma_0}{2}t} \sin(\omega_0 t) . \quad (4.30)$$

This regime has already been discussed at large in the literature also about QBs, typically employing a Lindblad master equation approach [117, 118, 187, 188]. Due to the small coupling, its charging performances are here very poor. Therefore we are not going to investigate it in the rest of the paper.

The second region is to the right of OD at large coupling $\gamma_0 \gg \omega_D, \omega_0$: it corresponds to a *strongly* UD (SUD) case. This region, has seldomly been discussed [189], however it presents a peculiar behavior which, as we will see, will play a fundamental role in the QB dynamics. Here we have (see App. D.2 for details)

$$\chi(t) \approx \frac{1}{\Omega} e^{-\frac{\omega_D}{2}t} \sin(\Omega t) . \quad (4.31)$$

As is clear, in this regime $\Omega = \sqrt{\gamma_0 \omega_D}$ takes the role of the new natural frequency of the QB. Notice that since the strong coupling $\gamma_0 \gg \omega_D, \omega_0$ implies $\Omega \gg \omega_D, \omega_0$, this frequency is strongly renormalized with respect to the bare one. In addition, its value is outside the band-width of the reservoir ($\Omega \gg \omega_D$). As we will see, this

point is crucial to achieve the best charging protocol, discussed in Fig. 4.1 since the reservoir is dynamically blockaded around the frequency Ω of the QB preventing the energy absorption. For this reason in the rest of the paper we will mainly focus on this regime showing that it indeed produces the best short time charging performances.

We close this Section commenting on the OD regime (red region), where $\chi(t)$ displays no oscillations. As a typical example we remind the leading order behaviour in ω_D , with $\gamma_0 > 2\omega_0$ (dashed-dotted line in the figure) [64, 175]

$$\chi(t) \approx \frac{e^{-\frac{\gamma_0}{2}t}}{\sqrt{(\gamma_0/2)^2 - \omega_0^2}} \sinh \left[t \sqrt{(\gamma_0/2)^2 - \omega_0^2} \right]. \quad (4.32)$$

Here, the dynamics of the QB is damped and it is not very useful for our purposes since the reservoir absorbs the main part of the incoming energy with an inefficient charging protocol similar to Fig. 4.1(b). For more details see the Supplementary Information of Ref. [36].

4.4 Main results

4.4.1 Relevant quantities

To study in details the charging dynamics we start by specifying the initial conditions. We assume that, prior to the charge phase, the QB and the reservoir are disconnected. In addition, we consider an initial Gaussian state with the QB in its ground state $|g\rangle$ and the reservoir in its thermal equilibrium at temperature T . This corresponds to a factorized initial density matrix $\rho(0) = \rho_B(0) \otimes \rho_R(0)$ with:

$$\rho_B(0) = |g\rangle\langle g|; \quad \rho_R(0) = \frac{e^{-\beta \hat{H}_R(0)}}{\text{Tr} \left\{ e^{-\beta \hat{H}_R(0)} \right\}}. \quad (4.33)$$

With this choice, the averages of position and momentum of both the QB and the reservoir variables are zero at $t = 0$, while the second moments are

$$\langle \hat{x}^2(0) \rangle = \frac{1}{2m\omega_0}, \quad \langle \hat{p}^2(0) \rangle = \frac{m\omega_0}{2}, \quad \langle \{ \hat{x}(0), \hat{p}(0) \} \rangle = 0 \quad (4.34)$$

for the QB, and

$$\langle x_k(0)x_{k'}(0) \rangle = \frac{1}{2m\omega_k} \coth(\beta\omega_k/2) \delta_{k,k'}, \quad (4.35)$$

$$\langle p_k(0)p_{k'}(0) \rangle = \frac{1}{2}m\omega_k \coth(\beta\omega_k/2) \delta_{k,k'}, \quad (4.36)$$

$$\langle \{x_k(0), p_{k'}(0)\} \rangle = 0 \quad (4.37)$$

for the reservoir. Due to these conditions the fluctuating noise $\xi(t)$ in Eq. (4.11) has zero average $\langle \hat{\xi}(t) \rangle = 0$ and time-translational invariant autocorrelation function [64]

$$\langle \hat{\xi}(t)\hat{\xi}(0) \rangle = \int_0^\infty \frac{d\omega}{\pi} J(\omega) \sum_{n=\pm 1} \frac{e^{in\omega t}}{2} \left[\coth\left(\frac{\beta\omega}{2}\right) - n \right]. \quad (4.38)$$

Since the initial density is Gaussian, all considerations reported in Section 2.2.3 about the ergotropy for a Gaussian states of an harmonic oscillator hold true. This is also due to the fact that the first moments remain equal to zero during the entire evolution, ensuring that the state is fully characterized by its second moments. All relevant quantities can be then evaluated knowing the covariance matrix $\sigma_B(t)$, given by Eq. (2.35). Much like the decomposition of $\hat{x}(t)$ into a homogeneous and thermal part, given in Eq. (4.12), the same holds for the covariance matrix: $\sigma_B(t) = \sigma_{B,h}(t) + \sigma_{B,th}(t)$ where the h (th) term only contains the homogeneous (thermal) contributions to $\langle \hat{x}^2(t) \rangle$ and $\langle \dot{\hat{x}}^2(t) \rangle$.

The homogeneous terms are easily written in terms of the response function

$$\begin{pmatrix} \langle \hat{x}_h^2(t) \rangle \\ \langle \dot{\hat{x}}_h^2(t) \rangle \end{pmatrix} = \frac{\omega_0}{2m} \begin{pmatrix} \chi^2(t) \\ \dot{\chi}^2(t) \end{pmatrix} + \frac{1}{2m\omega_0} \begin{pmatrix} \dot{\chi}^2(t) \\ \ddot{\chi}^2(t) \end{pmatrix}. \quad (4.39)$$

More cumbersome are the thermal contributions, which can be written in the compact form

$$\begin{pmatrix} \langle \hat{x}_{th}^2(t) \rangle \\ \langle \dot{\hat{x}}_{th}^2(t) \rangle \end{pmatrix} = \sum_{j,j'} \begin{pmatrix} 1 \\ \lambda_j \lambda_{j'} \end{pmatrix} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi m^2} \left\{ \frac{J(\omega) \coth\left(\frac{\beta\omega}{2}\right)}{(\lambda_j - i\omega)(\lambda_{j'} + i\omega)} \cdot \chi_j \chi_{j'} \left[1 - e^{-(\lambda_j - i\omega)t} - e^{-(\lambda_{j'} + i\omega)t} + e^{-(\lambda_j + \lambda_{j'})t} \right] \right\}. \quad (4.40)$$

More details on this are reported in App. D.3.

4.4.2 The underdamped strong coupling regime.

We can now study the charging/discharging protocol, at short times in the UD strong coupling regime, where the best performances as QB are achieved. All results are obtained numerically. However, we will also provide analytical expressions to support our results. In addition, we will focus on custom tailored reservoirs with quite small $\omega_D \gtrsim \omega_0$, with a narrow band and thus strongly non-Markovian, as this choice is one of the keys to obtain the best short-time performances among all the operating regimes.

A paradigmatic example

To begin our discussion, Fig. 4.3(a) shows the energy accumulated in the QB $\Delta E_B(t)$ (blue line), the energy delivered by the interaction Hamiltonian $\Delta E_{\text{int}}(t) = -W(t)$ (red line) and the energy dissipated into the reservoir $\Delta E_R(t)$ (green line) as a function of time, in the quantum regime $T = 0.1\omega_0$ for parameters within the SUD regime.

As is clear $\Delta E_B(t)$ shows oscillations with a period π/Ω , damped over a time scale ω_D^{-1} , and is locally maximum at times $t_n \approx \frac{\pi}{2\Omega} + n\frac{\pi}{\Omega}$, with $n \geq 0$ an integer. Notice that this energy is large: in particular, the maximum amount accumulated in the QB, occurring at the shortest time $t = t_0 \approx \pi/2\Omega$, is almost equal to $W_{\text{on}} = \Omega^2/4\omega_0$. These are already hints of a fast and extremely effective charging protocol. Notice that the oscillations of $\Delta E_B(t)$ are strikingly synchronized in phase opposition with

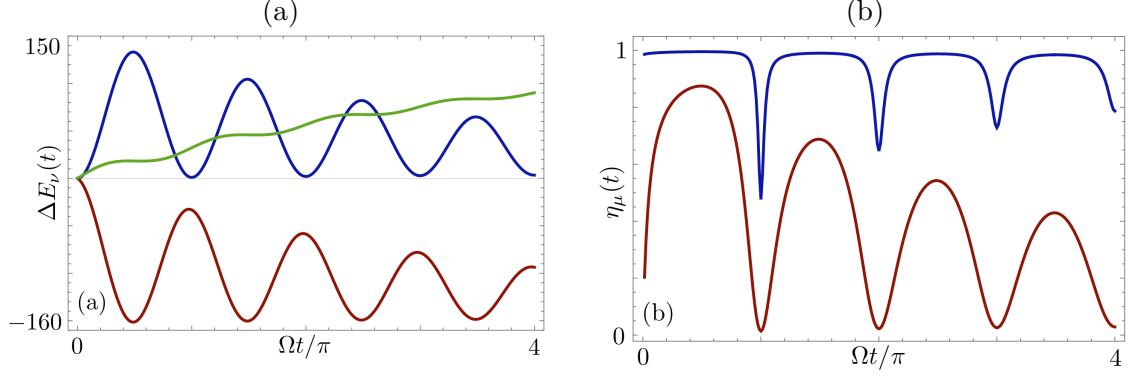


Figure 4.3: Panel (a) plot of $\Delta E_\nu(t)$ (units ω_0) with $\nu = \text{B}$ (blue curve), $\nu = \text{int}$ (red curve) and $\nu = \text{R}$ (green curve) as a function of $\Omega t/\pi$; panel (b) plot of $\eta_\mu(t)$ with $\mu = \text{B}$ (blue curve), and $\mu = \text{W}$ (red curve) as a function of $\Omega t/\pi$. Parameters are $\omega_D = 2\omega_0$, $\gamma_0 = 300\omega_0$ (corresponding to $\Omega \approx 24.5\omega_0$) and $T = 0.1\omega_0$. Image taken from [36] with minor modifications.

respect to $\Delta E_{\text{int}}(t)$, suggesting that at short times the charger and the QB almost perfectly exchange energy in lockstep. As a consequence, and as confirmed by the behavior of $\Delta E_{\text{R}}(t)$, during the first oscillations only a small fraction of energy is dissipated in the reservoir, whose dynamics seems to show an effective blockade at short times. We will turn back to this interpretation shortly. Concerning the state of the QB, as discussed in App. D.4, in correspondence of the first maxima we find it to be well described by a squeezed state strongly compressed along $\hat{x}$ and very elongated in the $\hat{p}$ direction. This observation could be in principle used as starting point to elaborate efficient protocols for energy extraction.

The extreme effectiveness of the protocol is definitively confirmed by the behavior of the efficiencies $\eta_{\text{B}}(t)$ and $\eta_{\text{W}}(t)$, shown in panel (b). Except around the minima of $\Delta E_{\text{B}}(t)$ we find $\eta_{\text{B}}(t) \sim 1$ which implies the best ergotropy $\mathcal{E}(t)$: almost equal to the energy stored in the QB. This in turns implies that almost all the energy accumulated in the QB can be effectively retrieved to produce useful work. Most importantly, however, $\eta_{\text{W}}(t)$ is excellent: around the first maximum it exceeds 0.85, and it is still very good around the fourth maximum where it reaches values above 0.5.

These results are indeed striking, especially in comparison with other similar charging-discharging protocols [149] that achieve significantly smaller values of $\eta_{\text{W}}(t)$. In this respect, one common critique of a fast charging/discharging protocol is the difficulty to fine-tune parameters in order to achieve the best performances [149]. However, in our scenario the almost perfect periodicity of all the quantities constitutes a key advantage: one is not forced to disconnect the QB from the charger at one peculiar time. Instead, the sequence of optimal times t_n is highly predictable with charging energies and, as we have seen and as will be shown later on, performances remaining remarkable (and thus, stable) over several oscillation periods.

To close this part, we turn back to interpret this optimal charging protocol in terms of a dynamical blockade of the reservoir. We remind that the reservoir is heavily structured with a small band-width ($\omega_D \ll \Omega$): this means that only the modes with $\omega_k \lesssim \omega_D \ll \Omega$ have a significant weight in the spectral density $J(\omega)$, see

Eqs. (4.21) and (4.22). However, these modes are completely off resonance with the QB and then we expect that they can hardly absorb energy, thus allowing a back and forth energy transfer between QB and charger.

To demonstrate this scenario we inspect the spectral contributions of the reservoir $\Delta E_R(t, \omega_k)$ defined in Eq. (4.19), or for more details see the Supplementary Information of Ref. [36]. Fig. 4.4(a) shows a density plot of $\Delta E_R(t, \omega_k)$, the dashed line represents the time window of Fig. 4.3. During the initial times the reservoir absorbs very little energy at all, due to the small value of the cut-off $\omega_D \ll \Omega$. This

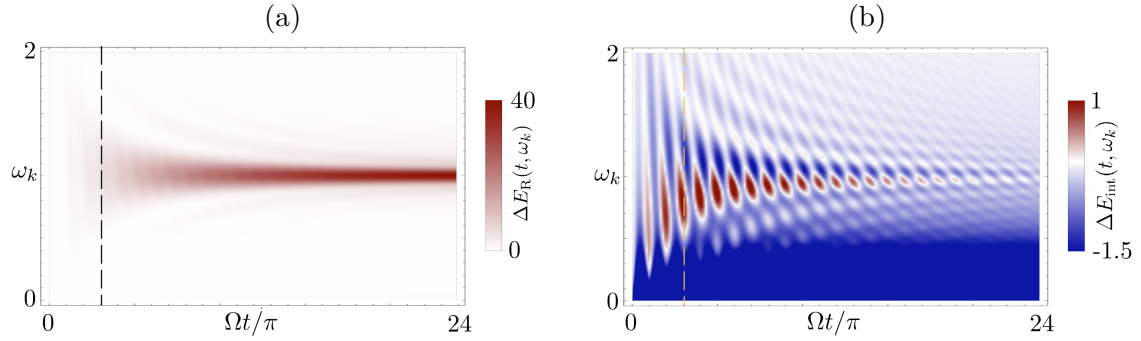


Figure 4.4: Spectral decomposition of the reservoir and coupling energies in the SUD regime. Density plots of (a) $\Delta E_R(t, \omega_k)$ and (b) $\Delta E_{\text{int}}(t, \omega_k)$, both in units Δ , as a function of $\Omega t/\pi$ and ω_k (units Ω). The dashed line represents the time window considered in Fig. 4.3. Here $\omega_D = 2\omega_0$, $\gamma_0 = 300\omega_0$ ($\Omega \approx 24.5\omega_0$) and $T = 0.1\omega_0$. Image taken from [36] with minor modifications.

allows the important process of energy exchange between the QB and the charger with anti-phase synchronization. This oscillating dynamics is clearly visible in the spectral contribution $\Delta E_{\text{int}}(t, \omega_k)$ of the charger, shown in panel (b), that oscillates between positive and negative values around $\omega_k = \Omega$. In particular the positive values signal that energy back-flows from the QB to the charger, since the energy in the reservoir slowly increases monotonically. On the other hand, away from the resonance $\Delta E_{\text{int}}(t, \omega_k) < 0$.

As time goes by, however, a sizeable amount of energy eventually accumulates into the reservoir: indeed the latter starts to respond revealing a clear resonance precisely around the modes with $\omega_k \approx \Omega$. As already pointed out, modes at such frequencies have a very small weight in $J(\omega)$ but still succeed to open a narrow "energy pathway" into the reservoir. In this time window the reservoir absorbs energy mainly at these frequencies, with all the other modes, including those at $\omega_k \lesssim \omega_D$, contributing sensibly less. Ultimately, the fact that energy flows considerably into the reservoir only for times $t > \frac{\pi}{\Omega}$, and essentially only via this narrow channel, strongly slows down damping which in turns boosts the charging performances, promoting the back-and-forth exchange of energy between the interaction Hamiltonian and the QB at short times.

Stability of the charging protocol

We will now study the stability of the above results with respect to variations of Ω and T , showing that very good performances are achieved even if we choose less

extreme parameters.

We begin by varying Ω , which we achieve by tuning γ_0 at fixed ω_D . Fig. 4.5 shows the results for $\omega_D = 2\omega_0$ and low temperature $T = 0.1\omega_0$. As can be seen, the qualitative behaviour is essentially unchanged within this wide range of Ω , and the best charging performances always occur at shortest times. As shown in panels (a) and (c), the energy accumulated in the QB and $\eta_B(t)$ increase for increasing Ω . This implies that at strong(er) coupling more useful energy ($\eta_B \rightarrow 1$) is stored in the QB. The almost out-of-phase behaviour of $\Delta E_B(t)$ and $\Delta E_{\text{int}}(t)$ is also confirmed, see panel (b). Also the efficiency $\eta_W(t)$, shown in panel (d), increases around the maxima for increasing coupling. It is even more important to observe, though, that even for the smallest value $\Omega \sim 7\omega_0$ considered here, very good performances around the first maximum are achieved with a very good maximum for $\eta_W(t)$ of about 0.6.

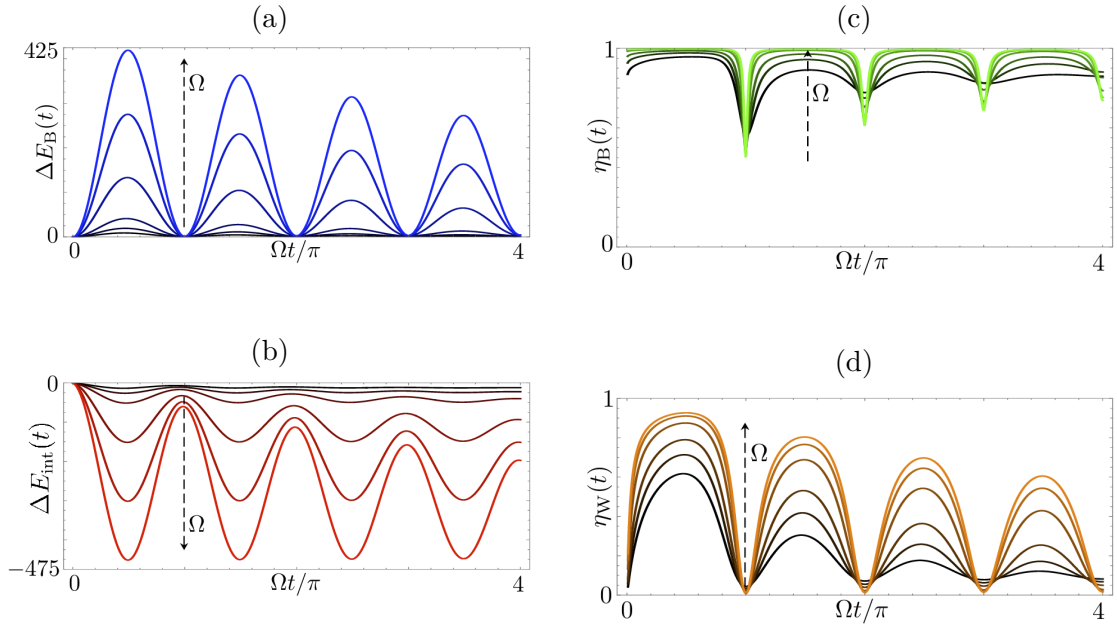


Figure 4.5: Plot of (a) $\Delta E_B(t)$ (units ω_0), (b) $\Delta E_{\text{int}}(t)$ (units ω_0), (c) $\eta_B(t)$, and (d) $\eta_W(t)$ as a function of $\Omega t/\pi$ for $\omega_D = 2\omega_0$ and different values of γ_0 : from black to color $\gamma_0 = 25\omega_0$ ($\Omega \approx 7.1\omega_0$), $50\omega_0$ ($\Omega = 10\omega_0$), $100\omega_0$ ($\Omega \approx 14.1\omega_0$), $300\omega_0$ ($\Omega \approx 24.5\omega_0$), $600\omega_0$ ($\Omega \approx 34.6\omega_0$) and $900\omega_0$ ($\Omega \approx 42.4\omega_0$). The dashed arrow marks the increasing direction of Ω . In all panels $T = 0.1\omega_0$. Image taken from [36] with minor modifications.

Concerning the effects of temperature, we show in Fig. 4.6 the results for the same parameters of Fig. 4.3 (SUD regime), for temperatures ranging from very low to high ones. As can be seen, the behavior of all the quantities of interest is essentially independent of the temperature and only when $T > \Omega$ deviations are found. In particular, notice that even though at the largest temperatures considered here $\eta_B(t)$ slightly decreases, its value around the maxima still is $\gtrsim 0.8$, which means that a high ergotropy can be retrieved from the QB even in this regime. Also, when $T > \Omega$ the oscillations of $\eta_W(t)$ tend to become slightly less pronounced as T increases, although we stress that the first maximum exhibits an exceptional resilience.

These results show a strong stability with respect to Ω and T . This leads to the

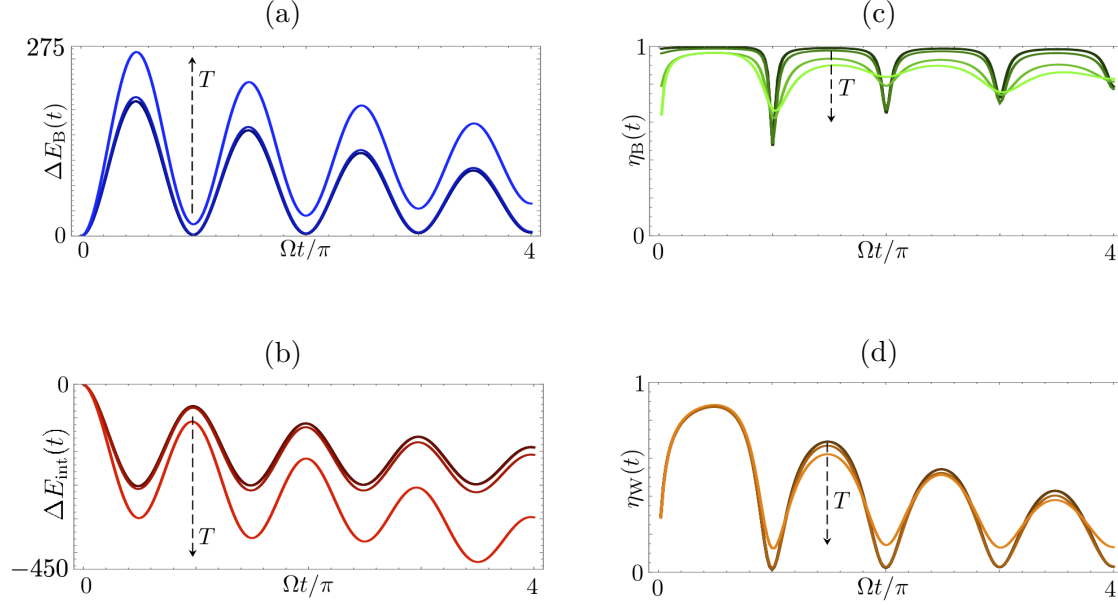


Figure 4.6: Plots of (a) $\Delta E_B(t)$ (units ω_0), (b) $\Delta E_{\text{int}}(t)$ (units ω_0), (c) $\eta_B(t)$, and (d) $\eta_W(t)$ as a function of $\Omega t/\pi$ for different values of T : from black to color $T = 0.1\omega_0$ ($T \approx 4 \cdot 10^{-3}\Omega$), ω_0 ($T \approx 4 \cdot 10^{-2}\Omega$), $10\omega_0$ ($T \approx 4 \cdot 10^{-1}\Omega$), $10^2\omega_0$ ($T \approx 4\Omega$), and $10^3\omega_0$ ($T \approx 40\Omega$). The dashed arrow marks the increasing direction of T . In all panels $\omega_D = 2\omega_0$ and $\gamma_0 = 300\omega_0$. Image taken from [36] with minor modifications.

important conclusion that our fast charge protocol is within reach of state of the art experimental platforms, without requiring exceedingly fast control or exceedingly low temperatures, see discussion about experimental feasibility in App. D.1.

Analytic results at short times

In the SUD regime, when $\Omega \gg \omega_D, \omega_0$ and in the short times limit $t \lesssim n\pi/\Omega$ (with $n > 1$ an integer of order unity), analytic expressions for $\langle \hat{\mathcal{H}}_B(t) \rangle$, the ergotropy and for the total work $W(t)$ can be obtained, that support our findings. Here we just quote the main results valid near the local maxima of $\Delta E_B(t)$, for details on the derivation see the Supplementary Information of Ref. [36].

At low temperature all quantities are dominated by homogeneous terms and one finds, to leading order in Ω , that

$$\langle \hat{\mathcal{H}}_B(t) \rangle \approx \langle \hat{\mathcal{H}}_B(t) \rangle_{\text{h}} ; \mathcal{E}(t) \approx \langle \hat{\mathcal{H}}_B(t) \rangle_{\text{h}} ; W(t) \approx W_{\text{h}}(t),$$

with

$$\langle \hat{\mathcal{H}}_B(t) \rangle_{\text{h}} = \frac{\Omega^2}{4\omega_0} e^{-\omega_D t} \sin^2(\Omega t). \quad (4.41)$$

Notice that in this regime the ergotropy is optimal, since it essentially matches the energy stored in the QB. One also has

$$W_{\text{h}}(t) = \frac{\Omega^2}{4\omega_0} [1 - e^{-\omega_D t} \cos^2(\Omega t)], \quad (4.42)$$

which allows to obtain a closed expression for the efficiency

$$\eta_W(t) = \frac{e^{-\omega_D t} \sin^2(\Omega t)}{1 - e^{-\omega_D t} \cos^2(\Omega t)}. \quad (4.43)$$

These equations provide results in excellent agreement with the numerical ones.

Conversely at high temperature ($T \gg \omega_D$) the energy of the QB, the ergotropy and the work acquire thermal contributions in addition to the homogeneous ones in Eqs. (4.41) and (4.42). We find $\langle \hat{\mathcal{H}}_B(t) \rangle = \langle \hat{\mathcal{H}}_B(t) \rangle_h + \langle \hat{\mathcal{H}}_B(t) \rangle_{th}$, with

$$\langle \hat{\mathcal{H}}_B(t) \rangle_{th} = \frac{T}{2} \left[e^{-\omega_D t} \sin^2(\Omega t) + (1 - e^{-\omega_D t}) \right]. \quad (4.44)$$

Concerning the total work $W(t) = W_h(t) + W_{th}(t)$, with

$$W_{th}(t) = \frac{T}{2} \left[e^{-\omega_D t} \sin^2(\Omega t) + \frac{\Omega^2}{\omega_0^2} \left(1 - e^{-\frac{2\omega_0^2 \omega_D t}{\Omega^2}} \right) \right]. \quad (4.45)$$

Comparing the additional thermal parts with respect to the homogeneous ones we see how the former become effectively dominant only for $T > \Omega$. The situation is slightly more complicated for the ergotropy $\mathcal{E}(t)$, since at high temperatures its expression deviates from that of $\langle \hat{\mathcal{H}}_B(t) \rangle_h$, see Fig. 4.6(c), signalling that the contribution of the covariance matrix becomes non negligible, see Eq. (2.34). One can still obtain an analytical expression for this quantity by evaluating the corrections due to the latter term starting from the approximated form of the variances (for details see the Supplementary Information of Ref. [36]). The final form is however too cumbersome to be reported. All the above expressions are in excellent agreement with our numerical results.

The long time limit

To close this Chapter, it is interesting to answer the question: what would happen, in the SUD regime, if one would defer the disconnection of the interaction Hamiltonian to very long times $t \rightarrow +\infty$? Notice that in this regime the reduced density matrix of the QB is given by the trace over the reservoir [64] $\rho_B(+\infty) = \text{Tr}_R \left\{ \frac{e^{-\beta \hat{\mathcal{H}}}}{Z} \right\}$, where $\hat{\mathcal{H}} = \hat{\mathcal{H}}_B + \hat{\mathcal{H}}_R + \hat{\mathcal{H}}_{int}$ the total Hamiltonian (see Eq. (4.1)) and with $Z = \text{Tr} \left\{ e^{-\beta \hat{\mathcal{H}}} \right\}$. Referring to the Supplementary Information of Ref. [36] for analytical details, here we quote the main results for both low and the high temperatures.

At low temperatures one finds $\langle \hat{\mathcal{H}}_B(+\infty) \rangle \approx \mathcal{E} \approx \frac{\Omega}{4}$ and $W(+\infty) \approx \frac{\Omega^2}{4\omega_0}$. Charging is still possible, and the ergotropy remains comparable with the energy stored in the QB. Observe however that in this case the latter quantity is proportional to Ω , while in the quick charge protocol outlined above the QB energy and ergotropy are of the order of Ω^2 , see Eq. (4.41). Thus, in this case much less energy can be effectively stored and retrieved. Even more importantly, in this regime charging requires a very large work so that one has $\eta_W(+\infty) \approx \omega_0/\Omega \ll 1$ and thus a much poorer efficiency with respect to the short-time performances.

In the high temperature regime ($T \gg \Omega$), dominated by energy equipartition, the situation is even worse. Indeed one finds $\langle \hat{\mathcal{H}}_B(+\infty) \rangle \approx T$ but, crucially, the ergotropy $\mathcal{E}$ scales as T^{-1} , implying $\eta_W(+\infty) \rightarrow 0$. This means that no useful work can be extracted from the QB: the charging is useless. Even more, also for other parameters the long-time performances never come even close to those obtained at short times in the SUD regime.

Chapter 5

Dicke quantum battery based on a Graphene Josephson Junction

In Section 2.4 we have described the Dicke QB as a representative model of a QB with a quantum charger [10, 128]. The aim of this Chapter is to present a possible solid-state realization of that model based on a JJ. Here the QB is composed of N TLSs, as in the standard Dicke model, but with a key difference: these TLSs are given by the different transport channels of the junction and the energy gaps are determined by their transmissions. Initially, the model is developed for a generic JJ, without specifying the microscopic details of the material. In a second stage, we focus on the specific case of a GJJ, where the transmission probabilities of the channels are derived from the electronic properties of graphene, a two-dimensional layers of carbon atoms [190–192]. This leads to a dispersion relation that characterizes the energy gaps of the TLSs forming the QB. Finally, we analyze the charging dynamics of the QB within this framework, highlighting the role of the graphene-induced spectral features in shaping the performance of the device. The results of this work will be published in Ref. [65].

5.1 Model

We consider a set up composed by a superconducting ring interrupted by a short superconductor-semiconductor hybrid JJ, which interacts inductively via a mutual inductance M with a superconducting resonator, as in the circuit shown in Fig. 5.1. In such hybrid JJ, the flow of a supercurrent is microscopically described in terms of pairs of Andreev Bound States (ABSs), which arise as a result of Andreev Reflections occurring at the superconductor-semiconductor interfaces [193]. They are subgap states, with energies symmetric around the Fermi level and smaller than the superconducting energy gap Δ_0 , which are spatially localized in the semiconducting region [194]. Moreover, the transport through the junction is characterized by the total number of available conduction channels N , which depends both on the microscopic properties of the semiconductor and on the geometry of the junction [195]. Within a Dirac–Bogoliubov–de Gennes (DBdG) approach [196], we consider a short and ballistic junction where the physical length of the junction channel L is much smaller than the superconductive coherence length ξ . According to this assumption, we can focus only on low-energy states. This electron system is described in terms

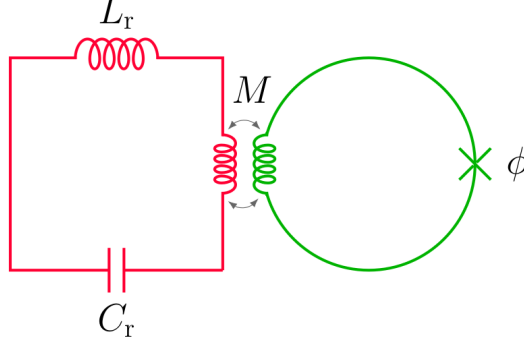


Figure 5.1: Schema of a Dicke QB based on a JJ. The charger is a resonant circuit (red) which is described as a lumped-element LC circuit with an inductance L_r and a capacitance C_r (see Section 1.2.3). The LC circuit is coupled, through a mutual inductance M , with a ring containing a single short hybrid JJ (green), which represents the QB. Here, ϕ represents the superconducting phase difference across the junction.

of pairs of ABSs with eigenenergies [197]

$$\pm \varepsilon_n(\phi) = \pm \Delta_0 \sqrt{1 - \tau_n \sin^2(\phi/2)}, \quad (5.1)$$

which depends on both the transmission probability of the n -th conduction channel with $n \in [1, N]$, τ_n , and on the superconducting phase difference ϕ across the junction [198]. Therefore, the system can be described as a collection of N non-interacting TLSs (given by the ABSs) with different energy splittings $2\varepsilon_n(\phi)$. For a given value of ϕ , by projecting the matter Hamiltonian in the low-energy subspace spanned by the ABSs [199], we can model the Hamiltonian of our QB as

$$\hat{\mathcal{H}}_B^{(JJ)} = \sum_{n=1}^N \varepsilon_n(\phi) \hat{\sigma}_n^z, \quad (5.2)$$

where each Pauli matrix $\hat{\sigma}_n^\nu$ ($\nu = x, y, z$) acts here on the two-dimensional subspace spanned by the n -th pair of ABSs. The QB Hamiltonian presents as ground-state (empty battery) and most excited eigenstate (completely full battery) the following two product states

$$|\downarrow\rangle \equiv \otimes_{n=1}^N |0\rangle_n, \quad |\uparrow\rangle \equiv \otimes_{n=1}^N |1\rangle_n, \quad (5.3)$$

respectively. In the charger-mediated protocol that we are considering, the auxiliary system, which plays the role of the charger, is a superconducting resonator [200, 201]. We model it as a lumped-element LC circuit with an inductance L_r and a capacitance C_r , following the standard quantization procedure described in Section 1.2.3 [169]. The Hamiltonian $\hat{\mathcal{H}}_C$ of the LC circuit is reported in Eq. (1.61), with $\Omega_{LC} = \omega_r = 1/\sqrt{L_r C_r}$. The interaction term that encodes the energy transfer between the two subsystems can be derived starting from the cQED formulation outlined in Refs. [202, 203], where is assumed that the flux quantum fluctuations in the LC circuit lead to an excess of flux through the ring and are responsible for the arising of a coupling λ between radiation (harmonic oscillator) and matter (ABSs)

degrees of freedom. Accordingly, the total Hamiltonian is obtained as a second order expansion with respect to the coupling

$$\hat{\mathcal{H}}_{\text{JJ}} = \hat{\mathcal{H}}_{\text{B}}^{(\text{JJ})} + \hat{\mathcal{H}}_{\text{C}} + \lambda(\hat{a} + \hat{a}^\dagger) \sum_{n=1}^N \mathbf{P}_n \cdot \hat{\boldsymbol{\sigma}}_n + \frac{\lambda^2}{2} (\hat{a} + \hat{a}^\dagger)^2 \sum_{n=1}^N \mathbf{D}_n \cdot \hat{\boldsymbol{\sigma}}_n, \quad (5.4)$$

where for brevity, we define $\hat{\boldsymbol{\sigma}}_n = (\hat{\sigma}_n^z, \hat{\sigma}_n^x)^1$ and

$$\begin{aligned} \mathbf{P}_n &= (P_n^z(\phi), P_n^x(\phi)) = \partial_\phi \varepsilon_n(\phi) \left(1, -\sqrt{1 - \tau_n} \tan\left(\frac{\phi}{2}\right) \right), \\ \mathbf{D}_n &= (D_n^z(\phi), D_n^x(\phi)) = \partial_\phi \varepsilon_n(\phi) \left(\frac{\tau_n + (2 - \tau_n) \cos(\phi)}{2 \sin(\phi)}, -\sqrt{1 - \tau_n} \right), \end{aligned} \quad (5.5)$$

with

$$\partial_\phi \varepsilon_n(\phi) = -\frac{\Delta_0 \tau_n \sin(\phi/2) \cos(\phi/2)}{2\sqrt{1 - \tau_n \sin^2(\phi/2)}}, \quad (5.6)$$

as vectors which encode the coupling terms with longitudinal and transverse components respectively. The third and fourth terms in Eq. (5.4) are the interaction Hamiltonian between the QB and the charger $\hat{\mathcal{H}}_{\text{int}}^{(\text{JJ})}$, and they are analogous to the paramagnetic and diamagnetic contributions typically emerging in an atomic light-matter coupling Hamiltonian [204]. Notice that a similar Hamiltonian, showing a two-photon coupling, has been recently discussed in the framework of Dicke QBs [120]. According to the definition in Eq. (2.8) and to the Hamiltonian in Eq. (5.2), the capacity of the QB is

$$\mathcal{C}_{\text{B}}^{(E)}(\phi) = \langle \uparrow | \hat{\mathcal{H}}_{\text{B}}^{(\text{JJ})} | \uparrow \rangle - \langle \downarrow | \hat{\mathcal{H}}_{\text{B}}^{(\text{JJ})} | \downarrow \rangle = 2 \sum_{n=1}^N \varepsilon_n(\phi), \quad (5.7)$$

where we emphasize the dependence on the superconducting phase difference to remark that this energy storage capacity can be controlled via the application of an external magnetic flux through the ring shown in Fig. 5.1. The total Hamiltonian in Eq. (5.4) does not present peculiar symmetries, henceforth we investigate the behavior of the QB, for a fixed number N of ABSs, employing a full numerical approach.

5.1.1 Transmission probabilities in a GJJ

As an example we study here a planar GJJ characterized by a length L , a finite width W and a chemical potential μ_0 , as shown in Fig. 5.2. The eigenvalue problem along the transverse direction in the normal graphene region can be solved by imposing the so-called infinite mass boundary conditions at $y = \{-W/2, +W/2\}$. According to Ref. [205], the quantization on the transverse wavenumbers leads to

$$q_j = \pi \frac{L}{W} \left(j + \frac{1}{2} \right), \quad j = 1, 2, \dots, \quad (5.8)$$

expressed in units of $1/L$, while the transmission probability in pristine monolayer graphene is [206]

$$\tau_j = \frac{k_{\text{F}}^2 - q_j^2}{k_{\text{F}}^2 - q_j^2 \cos^2(\sqrt{k_{\text{F}}^2 - q_j^2})} \quad (5.9)$$

¹Notice that this definition is different to the one used in Chapter 1.

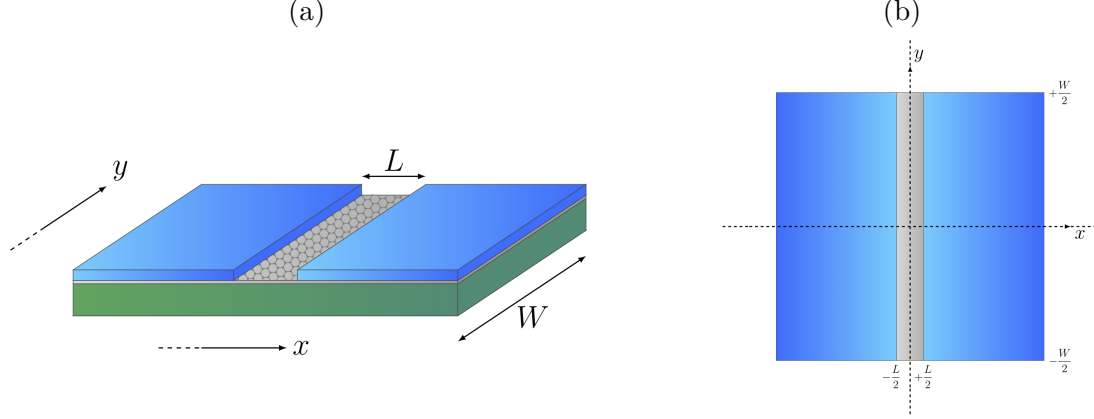


Figure 5.2: (a) Scheme of the JJ formed by a monolayer graphene (grey) covered by two superconducting leads (blue). The uncovered grey region represents the stripe in the normal phase. In this picture, L represents the junction channel length along the x -direction and W is the width of the device along the y -direction. (b) Planar view of the junction. The boundary conditions are imposed at $y = \pm W/2$.

where $k_F = |\mu_0|L/v_F$ is the dimensionless Fermi wavenumber with $v_F \sim c/300$ the Fermi velocity.

Note that we can now substitute the transmission probability in Eq. (5.9) in the ABSs spectrum in Eq. (5.1) with $L \ll \xi \sim v_F/\Delta_0$. The phase difference ϕ and the chemical potential μ_0 are the two tunable parameters of the device.

After quantizing the transverse wavenumber according to Eq. (5.8), the number of propagating modes, characterized by $|q_j| \leq k_F$, is given by

$$N_m = 2 \left\lfloor \frac{\mu_0 W}{\pi v_F} - 1/2 \right\rfloor, \quad (5.10)$$

where $\lfloor \cdot \rfloor$ indicates the integer part. Taking also into account the valley degree of freedom in graphene, $\zeta = \pm$, we obtain the following low-energy Hamiltonian

$$\hat{\mathcal{H}}_B = \sum_{\zeta=\pm} \sum_{j=1}^{N_m} \varepsilon_j(\phi) \hat{\sigma}_{\zeta,j}^z. \quad (5.11)$$

The valley degree of freedom is not involved in the interaction considered in Eq. (5.4), therefore it introduces only a double degeneracy in our model. In order to adapt this description to the single summation which appears in Eq. (5.2), we introduce a compact index $\nu = \zeta \times j$ which allows us to recast both Eq. (5.8) and Eq. (5.11) as

$$\hat{\mathcal{H}}_B = \sum_{\nu} \varepsilon_{\nu}(\phi) \hat{\sigma}_{\nu}^z, \quad q_{\nu} = \pi \frac{L}{W} \left(|\nu| - \frac{1}{2} \right), \quad \nu = \pm 1, \pm 2, \dots, \pm N_m. \quad (5.12)$$

Therefore where $N \equiv 2N_m$ is the total number of conduction channels that we assume characterize the transport in the GJJ. Then, Eq. (5.4) can be simply adapted to the case in Eq. (5.12) by coherently replacing the summations.

5.2 Results

5.2.1 Conventional charging protocol

The charging protocol that we will first analyze follows from what we have already considered in Section 2.4 [10, 61, 120, 128, 207] and consists in a sudden switching of the light-matter coupling in time as described by Eq. (2.96) [130–132]. As initial state for the charging process, we assume that the system is prepared in a factorized eigenstate of the Hamiltonian in Eq. (5.4) consisting of a Fock state of the resonator and the ground state for the matter part in Eq. (5.3), namely

$$|\Psi_0\rangle = |N\rangle \otimes |\downarrow\rangle, \quad (5.13)$$

analogous to the one defined in Eq. (2.99). Note that the Fock state contains a number of excitations equal to the number of conduction channels N , since the goal is to excite all the channels with the minimal number of photons.

Once the coupling is switched on, the Hamiltonian is the one reported in Eq. (5.4). In the following, we analyze the evolution of the energy stored in the QB, defined in Eq. (2.5), as a function of time and of the superconducting phase difference ϕ for some values of the coupling strength λ measured in units of $N\omega_r$, which represents the initial amount of energy inserted in the resonator. Therefore, the ratio $\Delta E_B^{(\lambda)}(t)/N\omega_r$ is a quantity that measures the fraction of energy that can be transferred from the charger to the QB during the charging process. In the contour plot in Fig. 5.3, $\Delta E_B^{(\lambda)}(t)/N\omega_r$ is shown as a function of the time and of the superconducting phase difference ϕ . In the weak coupling regime, in panel (a), it is possible to identify charging regions where the ratio $\Delta E_B^{(\lambda)}(t)/N\omega_r \geq 40\%$, around $\phi/\pi = 0.53$ (orange line) and $\phi/\pi = 0.59$ (red line), and also around $\phi/\pi = 0.76$, where a peak is visible, although less pronounced. From panel (c) it is evident that they are centered on the values of the superconducting phase difference for which the splitting energy 2ε of each ABS is in resonance, respectively, with ω_r (single-photon contribution) and $2\omega_r$ (two-photon contribution). Increasing the coupling strength (panel (b)), the behavior is both quantitatively and qualitatively different from the previous cases. From the quantitative point of view the absolute value of the normalized energy that it is possible to store in the QB increases, however in this case there are no evident resonances. To better explain this aspect, in the next Paragraph we report the spectral decomposition of the initial state $|\Psi_0\rangle$ over the eigenbasis $\{|\mathcal{E}_j\rangle\}$ of the total Hamiltonian $\hat{\mathcal{H}}_{JJ}$.

Spectral decomposition

In this Paragraph we indicate respectively with $\{\mathcal{E}_j\}$ and $\{|\mathcal{E}_j\rangle\}$ the eigenenergies and eigenstates, obtained by the numerical diagonalization of $\hat{\mathcal{H}}_{JJ}$ in Eq. (5.4). Under the unitary time evolution induced by this Hamiltonian, the state of the system $|\Psi\rangle$ at a time t will be

$$|\Psi(t)\rangle = e^{-i\hat{\mathcal{H}}_{JJ}t} |\Psi_0\rangle. \quad (5.14)$$

By inserting the resolution of the identity over the complete set $\{|\mathcal{E}_j\rangle\}$, we have that

$$|\Psi(t)\rangle = \sum_j e^{-i\mathcal{E}_j t} \langle \mathcal{E}_j | \Psi_0 \rangle |\mathcal{E}_j\rangle = \sum_j e^{-i\mathcal{E}_j t} c_j |\mathcal{E}_j\rangle. \quad (5.15)$$

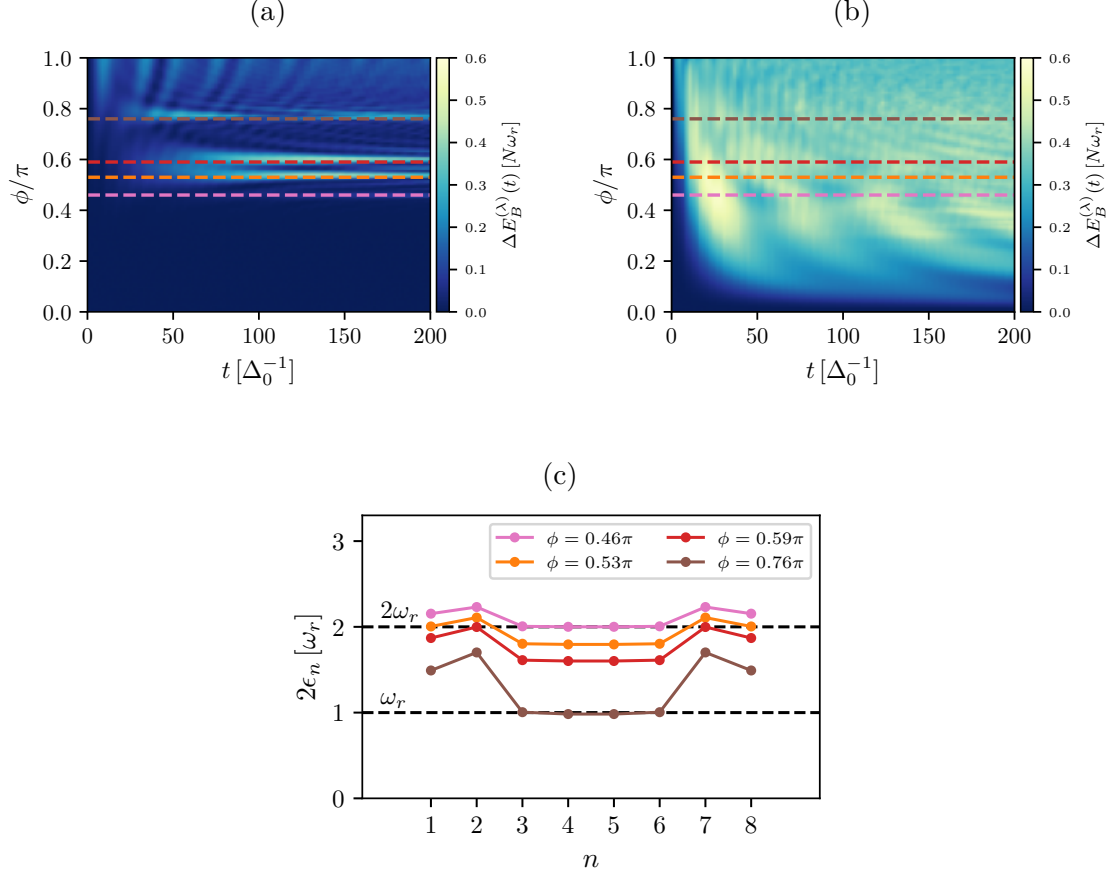


Figure 5.3: (a)-(b) Energy stored in the QB (in units of $N\omega_r$) using the charging protocol discussed in Eq. (2.96) as a function of t (in units of Δ_0^{-1}) and ϕ in (a) the weak ($\lambda = 0.1$) and (b) strong ($\lambda = 0.3$) coupling regime. The dashed lines correspond respectively to the partial resonances, highlighted in panel (c). (c) The splitting energy 2ϵ between each ABSs evaluated at $\phi/\pi = 0.46$ (pink line), $\phi/\pi = 0.53$ (orange line), $\phi/\pi = 0.59$ (red line), $\phi/\pi = 0.76$ (brown line). In all panels $\mu_0 = 6.5v_F/L$ and $W = 2L$, and $\omega_r = 0.75\Delta_0$

Since we are mainly interested in the expectation value of $\hat{\mathcal{H}}_B^{(JJ)}$ as a function of time, we can evaluate $E_B(t)$ using Eq. (2.4)

$$\begin{aligned}
 E_B(t) &= \left(\sum_s e^{i\mathcal{E}_s t} c_s^* \langle \mathcal{E}_s | \right) \hat{\mathcal{H}}_B^{(JJ)} \left(\sum_j e^{-i\mathcal{E}_j t} c_j | \mathcal{E}_j \rangle \right) = \\
 &= \sum_j |c_j|^2 \langle \mathcal{E}_j | \hat{\mathcal{H}}_B^{(JJ)} | \mathcal{E}_j \rangle + \sum_{s \neq j} \sum_j e^{-i(\mathcal{E}_j - \mathcal{E}_s)t} c_s^* c_j \langle \mathcal{E}_s | \hat{\mathcal{H}}_B^{(JJ)} | \mathcal{E}_j \rangle = \\
 &= \sum_j |c_j|^2 \langle \mathcal{E}_j | \hat{\mathcal{H}}_B^{(JJ)} | \mathcal{E}_j \rangle + \sum_{s \neq j} \sum_j e^{-i\Omega_{j,s} t} c_s^* c_j \langle \mathcal{E}_s | \hat{\mathcal{H}}_B^{(JJ)} | \mathcal{E}_j \rangle.
 \end{aligned} \tag{5.16}$$

If the fast-oscillating contributions, when $\Omega_{j,s} t \gg 2\pi$, dominate the second summation above, it is reasonable to expect that this second contribution is suppressed as a function of time. Since the set $\{\Omega_{j,s}\}$ represents all the possible splittings in the spectrum of $\hat{\mathcal{H}}_{JJ}$, the number of "large" splittings should increase if λ increases.

Therefore the condition

$$E_B \sim E_B^{static} = \sum_j |\langle \mathcal{E}_j | \Psi_0 \rangle|^2 \langle \mathcal{E}_j | \hat{\mathcal{H}}_B^{(JJ)} | \mathcal{E}_j \rangle \quad (5.17)$$

may be reached at short enough time. In Fig. 5.4 we report the tomography of the initial state $|\Psi_0\rangle$, that is the distribution of $|c_j|^2 = \langle \mathcal{E}_j | \Psi_0 \rangle|^2 \forall |\mathcal{E}_j\rangle$ of the Hamiltonian $\hat{\mathcal{H}}_{JJ}$. Panels (a) and (b) display the distribution of the coefficients c_j correspond-

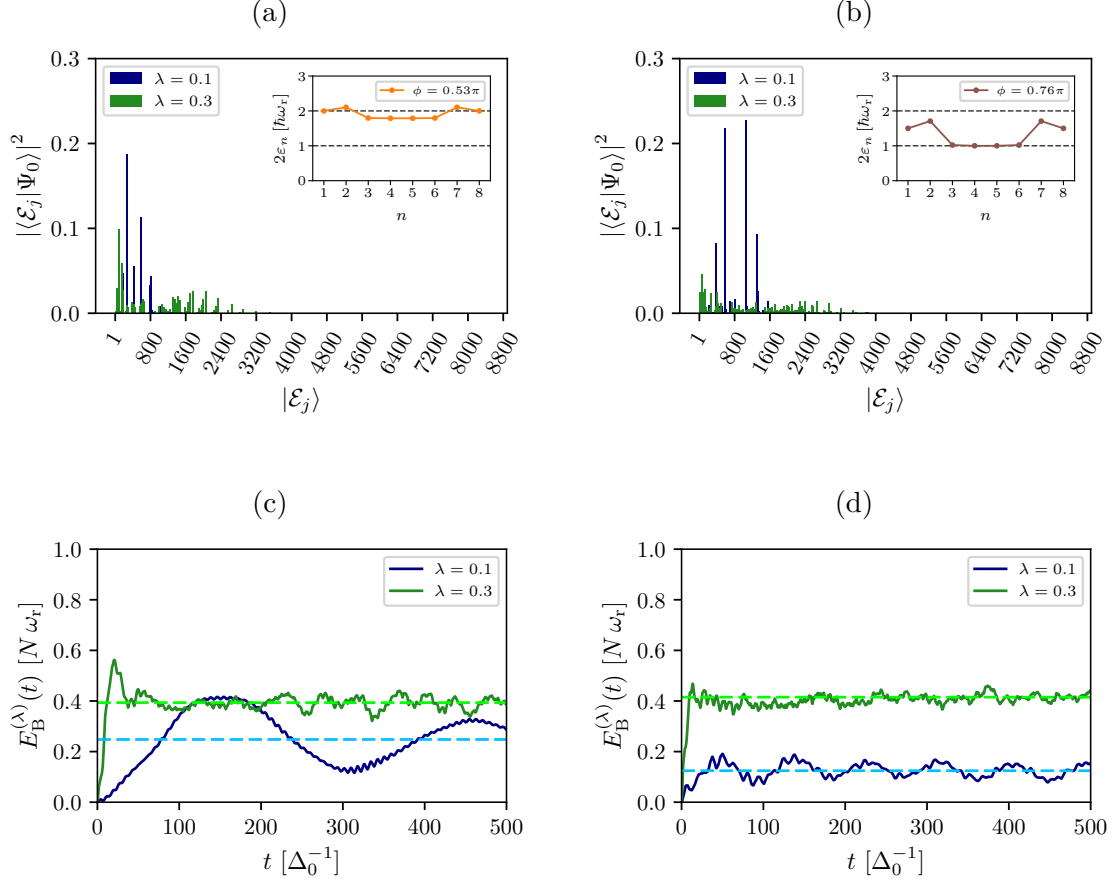


Figure 5.4: Decomposition of the initial state $|\Psi_0\rangle$ over the eigenbasis $\{|\mathcal{E}_j\rangle\}$ of the total Hamiltonian at $\phi/\pi = 0.53$ (a) and $\phi/\pi = 0.76$ (b), evaluated in the small coupling regime (blue) and the strong coupling regime (green). Comparison between the value of $E_{B,st}$ (dashed lines) and the time behaviour of the battery energy (solid lines) evaluated at $\phi/\pi = 0.53$ (c) and $\phi/\pi = 0.76$ (d).

ing to the single-photon and two-photon resonance conditions, respectively. The weak coupling regime is characterized by a spectrum dominated by a small number of discrete modes, whereas in the strong coupling regime the energy distribution spans over a larger set of modes. This difference is reflected in panels (c) and (d), which show the time evolution of the stored energy. In the weak coupling case, the dynamics exhibit pronounced oscillations governed by few dominant frequencies. Conversely, in the strong coupling regime, the presence of many contributing modes leads to a rapid convergence of the energy toward a stationary value.

This contrast explains the qualitatively different behaviors observed in Fig. 5.3, where resonant features emerge clearly in the weak coupling regime, and become suppressed in the strong coupling case.

5.2.2 Equal transmission probability

In this Section, we compare the situation described above with an ideal model described by a unique τ_{eq} , namely when the N conduction channels in the JJ are all characterized by the same effective transmission probability, obtained from a fit of the equilibrium supercurrent [199, 208], that can be written as

$$I(\phi) = 2e\langle\partial_\phi\hat{\mathcal{H}}_{\text{B}}\rangle_{\text{eq}} = 2e\sum_{\zeta=\pm}\sum_{j=1}^{N_{\text{m}}}\zeta\partial_\phi\varepsilon_n(\phi)n_{\text{F}}(\zeta\varepsilon_j(\phi)) \quad (5.18)$$

with $n_{\text{F}}(E)$ the Fermi-Dirac distribution. This is typically the case for ballistic superconductor–normal-metal–superconductor JJs [209, 210]. Notice that with this simplification the model reduce to an homogeneous Dicke model showing single- and two-photon interaction [211, 212].

At $t = 0^-$, the total Hamiltonian is

$$\hat{\mathcal{H}}_0 = \omega_{\text{r}}\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) + \varepsilon(\phi)\sum_n\hat{\sigma}_n^z, \quad (5.19)$$

and represents N TLSs equally splitted in energy, decoupled from the resonator. We assume that the system is prepared in the same state defined in Eq. (5.13). Once the coupling is switched on, the interaction part in total Hamiltonian in Eq. (5.4) becomes uniform

$$\hat{\mathcal{H}}_{\text{JJ}}^{(e)} = \hat{\mathcal{H}}_0 + \lambda(\hat{a} + \hat{a}^\dagger)\mathbf{P} \cdot \sum_{n=1}^N\hat{\boldsymbol{\sigma}}_n + \frac{\lambda^2}{2}(\hat{a} + \hat{a}^\dagger)^2\mathbf{D} \cdot \sum_{n=1}^N\hat{\boldsymbol{\sigma}}_n, \quad (5.20)$$

and the initial state undergoes a unitary evolution. In complete analogy with the previous Section, in the following we analyze the evolution of the energy stored in the QB measured in units of $N\omega_{\text{r}}$. In the contour plot in Fig. 5.5(a), $\Delta E_{\text{B}}^{(\lambda)}(t)/N\omega_{\text{r}}$ is shown as a function of time and of the superconducting phase difference ϕ . It is possible to identify features similar to the ones shown in Fig. 5.3. Here we have two charging regions where the ratio $\Delta E_{\text{B}}^{(\lambda)}(t)/N\omega_{\text{r}} \geq 60\%$, around $\phi/\pi = 0.82$ (orange line) and $\phi/\pi = 0.48$ (pink line). From Fig. 5.5(c) it is evident that they are centered on the values of the superconducting phase difference for which the splitting energy 2ε of each ABS is in resonance, respectively, with ω_{r} and $2\omega_{\text{r}}$. This further strengthens the analysis carried out in the previous Section and indicates that the performances of a real GJJ QB are not that far from what is obtained in the ideal case. To better understand the behavior of the system in the two optimal charging regions, in the following we address time evolution of the energy around $\phi/\pi = 0.48$ and $\phi/\pi = 0.82$.

Short time approximation

Here we show the behavior of the system in the two charging regions highlighted in Fig. 5.5. At $t = 0^-$, the total Hamiltonian is $\hat{\mathcal{H}}_0$ in Eq. (5.19) and the initial state

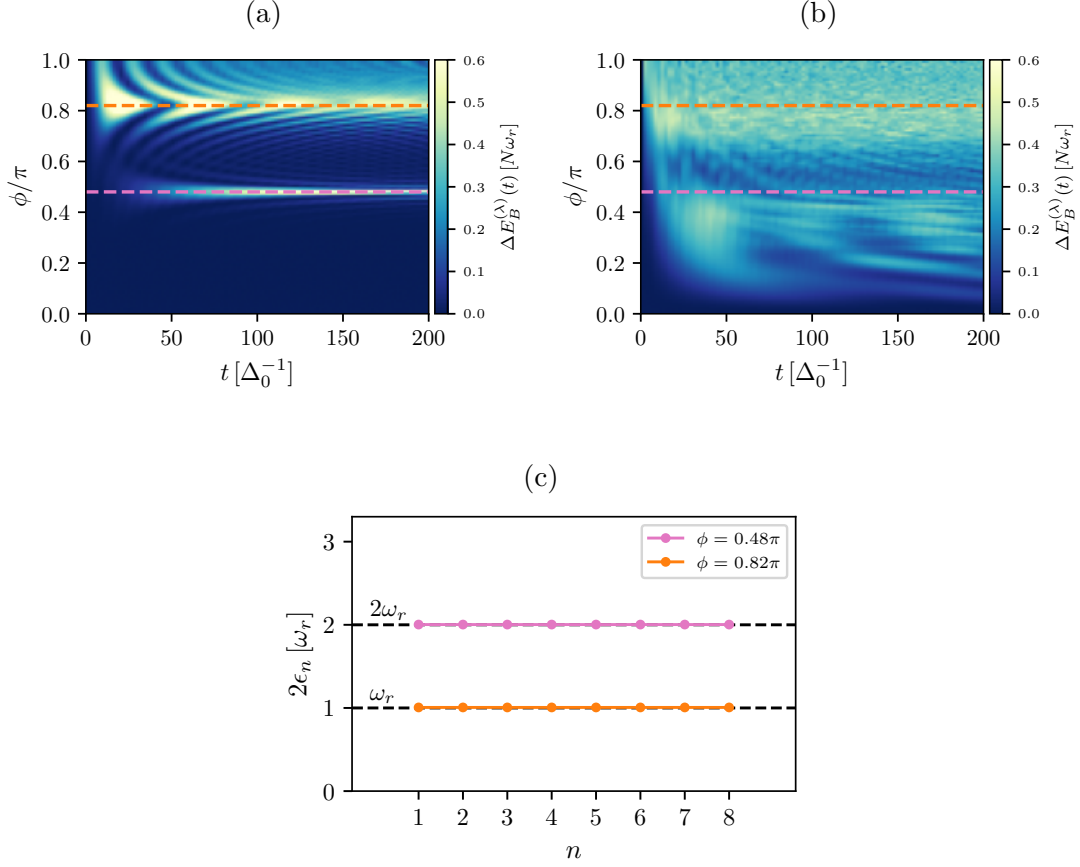


Figure 5.5: Energy stored in the QB (in units of $N\omega_r$) using the charging protocol discussed in Eq. (2.96), and as a function of t (in units of Δ_0^{-1}) and ϕ in (a) the weak ($\lambda = 0.1$) and (b) strong ($\lambda = 0.3$) coupling regime. The dashed lines correspond respectively to the resonances, highlighted in panel. (c). (c) The splitting energy 2ϵ between each ABSs evaluated at $\phi/\pi = 0.48$ (pink line) and $\phi/\pi = 0.82$ (orange line). Other parameters are $\tau_{eq} = 0.93$, $N = 8$, $\omega_r = 0.75\Delta_0$.

is the one in Eq. (5.13). For $t \in [0^+, t_C]$, the Hamiltonian is $\hat{\mathcal{H}}_{JJ}$ in Eq. (5.20). In the optimal charging regions, all splittings are in resonance with the single-photon energy

$$2\epsilon(\phi_{1ph}) = 2\Delta_0 \sqrt{1 - \tau_{eq} \sin^2(\phi_{1ph}/2)} \equiv \omega_r \quad (5.21)$$

or with the two-photon energy

$$2\epsilon(\phi_{2ph}) = 2\Delta_0 \sqrt{1 - \tau_{eq} \sin^2(\phi_{2ph}/2)} \equiv 2\omega_r. \quad (5.22)$$

We evaluate the time dependence of the energy stored in the QB induced by Eq. (5.20). Blue curves in Fig. 5.6 show the evolution of the energy around $\phi/\pi = 0.48$ and $\phi/\pi = 0.82$.

We can derive an approximate Hamiltonian that successfully reproduces the

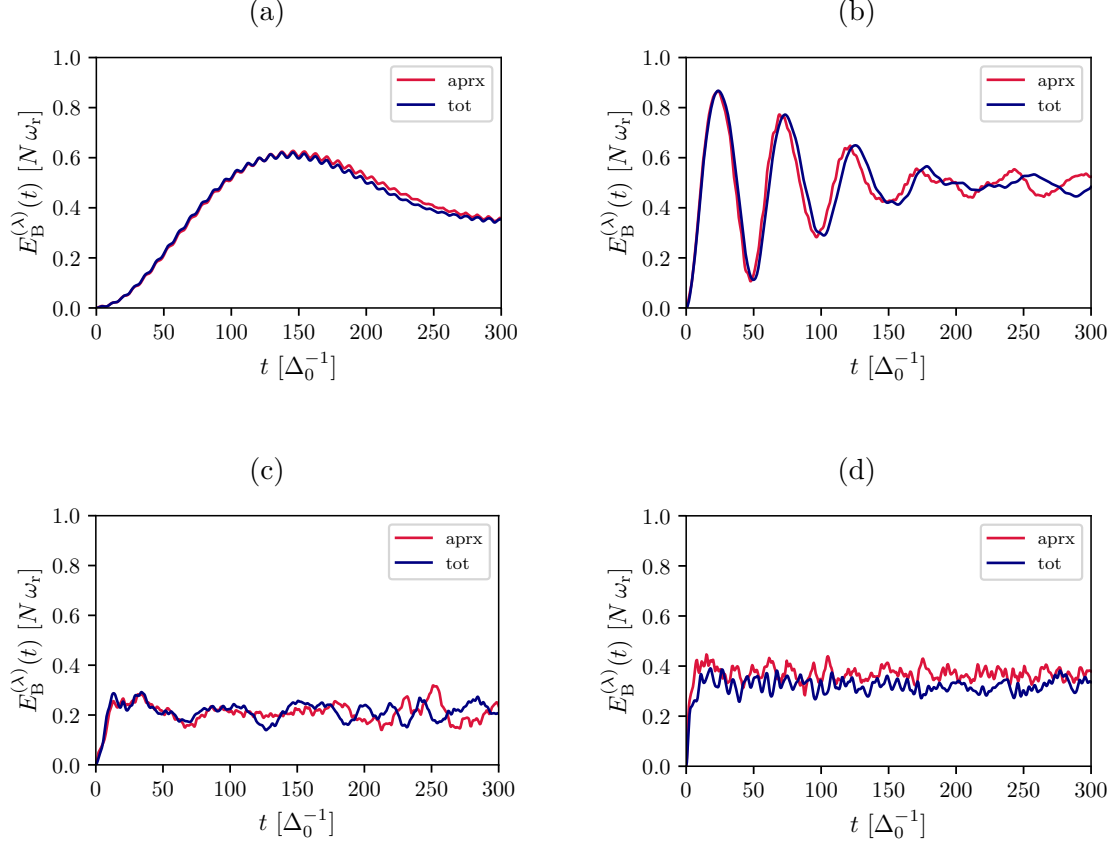


Figure 5.6: Energy stored in the QB (in units of $N\omega_r$) using the conventional charging protocol discussed in Eq. (2.96) (blue curves), as a function of t (in units of Δ_0^{-1}), compared to the result of the evolution generated by the approximated Hamiltonian in Eq. (5.23) (red curves). We show the result for $\phi/\pi = 0.48$ (a), (c) and for $\phi/\pi = 0.82$ (b), (d). The first row represents the small ($\lambda = 0.1$) coupling regime, while the second row the strong ($\lambda = 0.3$) one. Other parameters are $\tau_{eq} = 0.93$, $N = 8$, $\omega_r = 0.75\Delta_0$.

numerical dynamics, at least for short enough times. The expression is given by

$$\begin{aligned}
 \hat{\mathcal{H}}_{\text{aprx}} = & \omega_r \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \left(1 + \frac{\lambda^2}{\omega_r} D_z(\phi) \sum_n \hat{\sigma}_n^z \right) + \varepsilon(\phi) \sum_n \hat{\sigma}_n^z + \\
 & + \lambda P_z(\phi) (\hat{a} + \hat{a}^\dagger) \sum_n \hat{\sigma}_n^z + \lambda P_x(\phi) \sum_n [\hat{a} \hat{\sigma}_n^+ + \hat{a}^\dagger \hat{\sigma}_n^-] + \\
 & + \frac{\lambda^2}{2} D_x(\phi) \sum_n [(\hat{a})^2 \hat{\sigma}_n^+ + (\hat{a}^\dagger)^2 \hat{\sigma}_n^-],
 \end{aligned} \tag{5.23}$$

Numerical analysis shows that the first term on the second line of this equation is crucial to accurately capture the system's behavior within the considered coupling range, $\lambda = 0.100 - 0.300$. In particular, this term appears to limit the battery charging efficiency in the upper part of the λ range, where counter-rotating contributions also begin to significantly affect the energy transfer process.

5.2.3 Alternative charging protocol

Although the protocol in Eq. (2.96) has been considered in various theoretical works [7–22], it is challenging actually to implement it in scalable architectures [14, 213], due to the need of introducing quantum couplers [130–132]. As an alternative proposal, the second charging protocol we discuss in this work relies on the dependence on the superconductive phase difference of the ABSs spectrum. It consists of a sudden switching of the superconductive phase difference across the JJ

$$\phi(t) = \phi_0 \theta(t) \theta(\bar{t} - t) \quad (5.24)$$

that, despite challenging, can be achieved in cQED apparatus [214]. This opens the possibility to effectively couple (decouple) light and matter degrees of freedom by the decreasing (increasing) of the detunings between their characteristic energies. In this case, our initial Hamiltonian reads

$$\hat{\mathcal{H}}_{\text{JJ}}(t = 0^-) = \omega_r \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) + \Delta_0 \sum_n \hat{\sigma}_n^z + \frac{\lambda^2}{2} (\hat{a} + \hat{a}^\dagger)^2 \left[-\frac{\Delta_0}{4} \sum_n \tau_n \hat{\sigma}_n^z \right]. \quad (5.25)$$

We notice that the following commutation relations are fulfilled

$$[\hat{\sigma}_m^z, \hat{\sigma}_n^z] = 0 \quad \forall m, n \longrightarrow [\hat{\mathcal{H}}_{\text{JJ}}(t = 0^-), \hat{\sigma}_n^z] = 0 \quad \forall n. \quad (5.26)$$

As a consequence, the Hamiltonian in Eq. (5.25), can be diagonalized exactly for each initial set $\{s_n^z = \pm 1\}$ of the z -components of these fictitious spins, since it is a conserved quantity. We write the Hamiltonians as a functional of this set $\{s_n^z\}$

$$\hat{\mathcal{H}}_{\text{JJ}}(t = 0^-) = \hat{\mathcal{H}}_s = \omega_r \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) + \varepsilon_0 + \frac{\lambda^2}{2} (\hat{a} + \hat{a}^\dagger)^2 \mathcal{D}_0, \quad (5.27)$$

where

$$\begin{aligned} \varepsilon_0 &= \Delta_0 \sum_n s_n^z, \\ \mathcal{D}_0 &= -\frac{\Delta_0}{4} \sum_n \tau_n s_n^z. \end{aligned} \quad (5.28)$$

It can be diagonalized via the following Bogoliubov-Valatin transformations

$$\begin{pmatrix} \hat{b} \\ \hat{b}^\dagger \end{pmatrix} = \begin{pmatrix} \cosh(x) & \sinh(x) \\ \sinh(x) & \cosh(x) \end{pmatrix} \begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix}, \quad [\hat{b}, \hat{b}^\dagger] = 1, \quad (5.29)$$

where

$$x = \frac{1}{2} \ln(\varkappa), \quad \varkappa = \left[1 + \frac{2\lambda^2 \mathcal{D}_0}{\omega_r} \right]^{1/2}. \quad (5.30)$$

Therefore we have that

$$\hat{\mathcal{H}}_s = \varkappa \omega_r \left(\hat{b}^\dagger \hat{b} + \frac{1}{2} \right) + \varepsilon_0, \quad (5.31)$$

with a new vacuum state defined by the condition

$$\hat{b} |0\rangle_b = 0. \quad (5.32)$$

For $0^+ \leq t \leq \bar{t}$, i.e. $\phi(t) = \phi_0$, one has that the total Hamiltonian reads as

$$\begin{aligned} \hat{\mathcal{H}}_{\text{JJ}} = & \kappa\omega_r \left(\hat{b}^\dagger \hat{b} + \frac{1}{2} \right) + \sum_n \varepsilon_n(\phi) \hat{\sigma}_n^z \\ & + (\kappa^{1/2}\lambda)(\hat{b} + \hat{b}^\dagger) \sum_n [P_n^z(\phi) \hat{\sigma}_n^z + P_n^x(\phi) \hat{\sigma}_n^x] + \\ & + \frac{(\kappa^{1/2}\lambda)^2}{2} (\hat{b} + \hat{b}^\dagger)^2 \sum_n [(D_n^z(\phi) \hat{\sigma}_n^z - D_{n,0}^z s_n^z \mathbb{I}_n) + D_n^x(\phi) \hat{\sigma}_n^x], \end{aligned} \quad (5.33)$$

The new initial state is then

$$|\psi_0\rangle_b = |N\rangle_b \otimes |\downarrow\rangle. \quad (5.34)$$

Fig. 5.7 show the difference between the energy stored in the QB according to the two proposed protocols. The performance of the two charging protocols is remark-

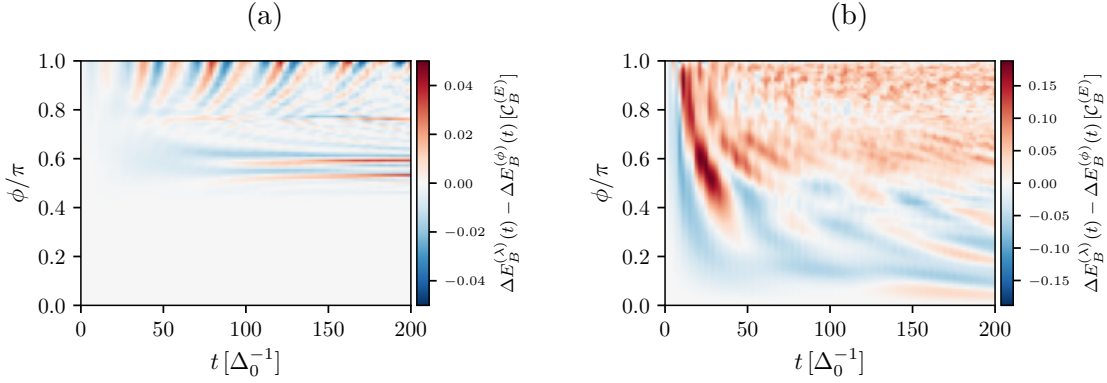


Figure 5.7: Difference between the energy stored in the QB (in units of the battery capacity $\mathcal{C}_B^{(E)}$) according to the conventional charging protocol ($\Delta E_B^{(\lambda)}(t)$) and to the alternative protocol ($\Delta E_B^{(\phi)}(t)$) as a function of t (in units of Δ_0^{-1}) and ϕ in the (a) weak ($\lambda = 0.1$) and (b) strong ($\lambda = 0.3$) coupling regime.

ably similar. However, the newly proposed scheme appears easier to implement experimentally [215–217], at least in principle, and offers a new direction for exploration in QB design. From a quantitative perspective, the difference between the two protocols remains modest in the weak coupling regime, only a few percent when normalized to the battery capacity. This regime is particularly interesting due to the presence of well-defined single- and two-photon resonances, which play a central role in the energy transfer dynamics, as discussed above. In these regions, where the amount of energy that can be stored is enhanced, this alternative protocol performs slightly better than the conventional one (blue areas), further highlighting its potential advantages. In contrast, under strong coupling conditions, the discrepancy becomes more pronounced, reaching approximately 10%. Moreover, in this regime, the regions of parameter space where the new protocol shows an advantage over the conventional one tend to be broader and more pronounced, suggesting a potential for improved performance under suitable conditions.

Conclusions & Perspectives

Although they have entered the scientific landscape only in the last decade, QBs have already taken on a central role in the domain of quantum technologies. Research in this field has mainly developed from a theoretical perspective, but recently the first experimental tests have appeared, allowing for greater optimism about possible future developments. To facilitate the transition from theoretical studies to practical applications, much of the current research activity is focused on models based on systems that could also be implemented experimentally.

This thesis fits precisely within this context. In the following, we present the concluding remarks, summarizing the key findings and their implications.

In Chapter 3 we studied the concept of a cyclic QB, operating according to a given thermodynamic cycle. During the whole cycle, the setup is weakly interacting with a thermal bath, while the operations are carried out on timescales shorter than those of the thermalization. This guarantees that the only role played by the reservoir is to reinitialize the system to the same thermal state at the end of every cycle. Our proposal for a QB is based on two connected qubits, whose non-trivial correlations, together with phase coherence, can be exploited to improve the performance of the device. A key outcome of this work is that the efficiency of the setup in the case of parallel energy extraction from two qubits can exceed the one where global operations are performed. Since local unitary operations are typically easier to implement than global ones, this result provides fertile ground for future implementations of such a kind of QB. Additionally, we simulated the proposed thermodynamic cycle on an IBM quantum hardware. The simulation on a quantum computer required to overcome several technical challenges, such as the realization of a given initial thermal state for the QB and error mitigation. The former was tackled with the introduction of thermofield double states, while a Bayesian optimization procedure was needed to deal with the latter. Despite unavoidable errors, mainly caused by the intrinsic noise in the device and by the probabilistic nature of the measurements, the obtained results foster the implementation of a cyclic QB using solid-state platforms. We also provided a minimal feasible scheme for a superconducting QB based on coupled charged qubits which can be recharged following the proposed thermodynamic cycle. The major advantage of experimental schemes of this type is their scalability, which leads to an enhancement of the overall storage capacity of the device.

In Chapter 4 we have proposed a scheme for a QB based on a quantum harmonic oscillator, strongly coupled to a non-Markovian reservoir via a quantum charger. The considered procedure relies on the transient dynamics which occurs right after the battery is connected to the quantum charger, thus ensuring a quick charging protocol. We have shown that the evolution of the energy stored in the battery is almost periodic, which allows to avoid a too precise fine-tuning of the time at which

the battery need to be disconnected from the charge. Moreover, we have shown that this protocol is very efficient, allowing in principle to extract through unitary operations almost all the energy stored in the QB, with a ratio between the energy that can be extracted and the work done by the charger which approaches the ideal unit limit. These features are due to two key ingredients, namely the non-Markovianity of the reservoir introduced by a spectral density with a cut-off of the order of the oscillator frequency, and a peculiar, and as yet almost unexplored, working regime characterized by a strong coupling between charger and QB. Crucially, these result in a dynamical blockade of the reservoir dynamics, allows an almost coherent exchange of energy between the charger and the QB at short enough times. Such model of QB may be realized with a quantum LC circuit playing the role of the battery and with the required environment being suitably engineered via state-of-the-art quantum circuits.

In Chapter 5 we have proposed a possible solid-state realization of the Dicke QB, based on a JJ. Starting from a general framework without specifying microscopic details, we then focused on the specific case of a GJJ, exploiting the electronic properties of graphene to determine the transmission probabilities of the transport channels. This approach enabled to derive a dispersion relation that defines the energy gaps of the TLSs composing the battery. The analysis of the charging dynamics highlighted how this more realistic model, designed with experimental feasibility in mind, achieves performance comparable to that of the standard Dicke model. This confirms that the proposed approach is not only theoretically sound but also a promising direction for future research and development in quantum technologies.

In the next years, QBs are expected to play an essential role in the development of quantum technology, improving the efficiency of energy distribution across complex quantum systems. In this framework, energy network and a detailed understanding of the thermodynamic cost associated with key operations are central areas of investigation. As in many field, artificial intelligence is expected to give a boost to research in this direction. Machine learning techniques could optimize charging and discharging protocols, and help to adapt performance to real-world conditions marked by noise and disorder. In conclusion, QBs are not just a new use of quantum mechanics, they represent a major change in how we think about and control energy at the quantum level. As research progresses, these devices are likely to become key to improve the speed, efficiency, and growth of quantum technologies. Thanks to advances in theory, experiments, and engineering, QBs are on track to become a major actor of the second quantum revolution.

Appendix A

Calibration and data analysis for the two/three level QB

The reconstruction of the state of a transmon, after the application of a time dependent external drive, is done through a readout in the so-called dispersive regime. Here, a harmonic oscillator (LC circuit playing the role of a resonator, see Section 1.2.3) is weakly coupled to the transmon and off-resonant with respect to it [105]. In this regime the frequency of the oscillator depends of the state of the transmon. This allows for a so called non-destructive measurement [218] based on the fact that a monochromatic microwave with frequency Ω_0 applied to the resonator is modified in such a way that

$$\cos \Omega_0 t \rightarrow A \cos(\Omega_0 t + \chi), \quad (\text{A.1})$$

with A and χ real numbers representing an amplitude and a phase respectively. Taking into account the complex representation of the transmitted wave at a given time, one can write

$$Ae^{i\chi} = I + iQ, \quad (\text{A.2})$$

with I and Q real numbers. Every measurement of the transmon state is therefore reported as a point in the (I, Q) plane. In order to accumulate proper statistics, the machine performs multiple runs (1024 in default settings). They are typically very scattered, requiring a further analysis to extract meaningful information from them. We have classified the points according to the three relevant states of the system ($|0\rangle$, $|1\rangle$ and $|2\rangle$) by means of scikit-learn, an open source machine learning library based on the Python programming language [219]. We have used support vector machines method with linear kernel function. This method takes as input two arrays: an array X of shape $(n_samples, n_features)$ holding the training samples, and an array y of class labels, that can be strings or integers, of shape $(n_samples)$. In our case we have 3072 samples with 2 features, I and Q and 3 possible labels, 0, 1 or 2. After being trained, the model can be used to classify new values.

Figure A.1 shows an example of data distribution with the coloured regions graphically representing the data labels. According to this picture, the energy stored in a qutrit QB (with respect to the ground state), can be determined through the relation

$$E(\eta) = \Delta \mathcal{P}_1(\eta) + \Delta_{max} \mathcal{P}_2(\eta) \quad (\text{A.3})$$

with

$$\mathcal{P}_i(\eta) = |\langle \Psi(\eta) | i \rangle|^2 \quad (\text{A.4})$$

and $\eta = \varphi_m, \Theta_m$ depending on the considered charging protocol.

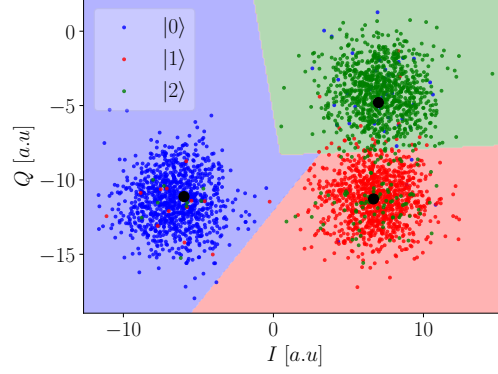


Figure A.1: Example of data distribution associated to the measurements of the state $|0\rangle$ (blue dots), $|1\rangle$ (red dots) and $|2\rangle$ (green dots) in the (I, Q) plane (in arbitrary units) for the `ibm_auckland` device. Big black dots indicate the centers of the different distributions, while straight lines separates the regions associated to every state. The efficiency of the considered separation is roughly 95.5% for the ground state, 95.7% for the first excited state and 90.0% for the second excited state. For each state shown in the plot, we have considered 1024 runs (3072 in total).

In figures A.2 and A.3 we show the different evolution of the state of the qutrit in the (I, Q) plane considering the sequential and simultaneous charging respectively. In particular, while in the former case there is an intermediate situation in which the system is in the state $|1\rangle$ with high probability, this doesn't happens in the latter.

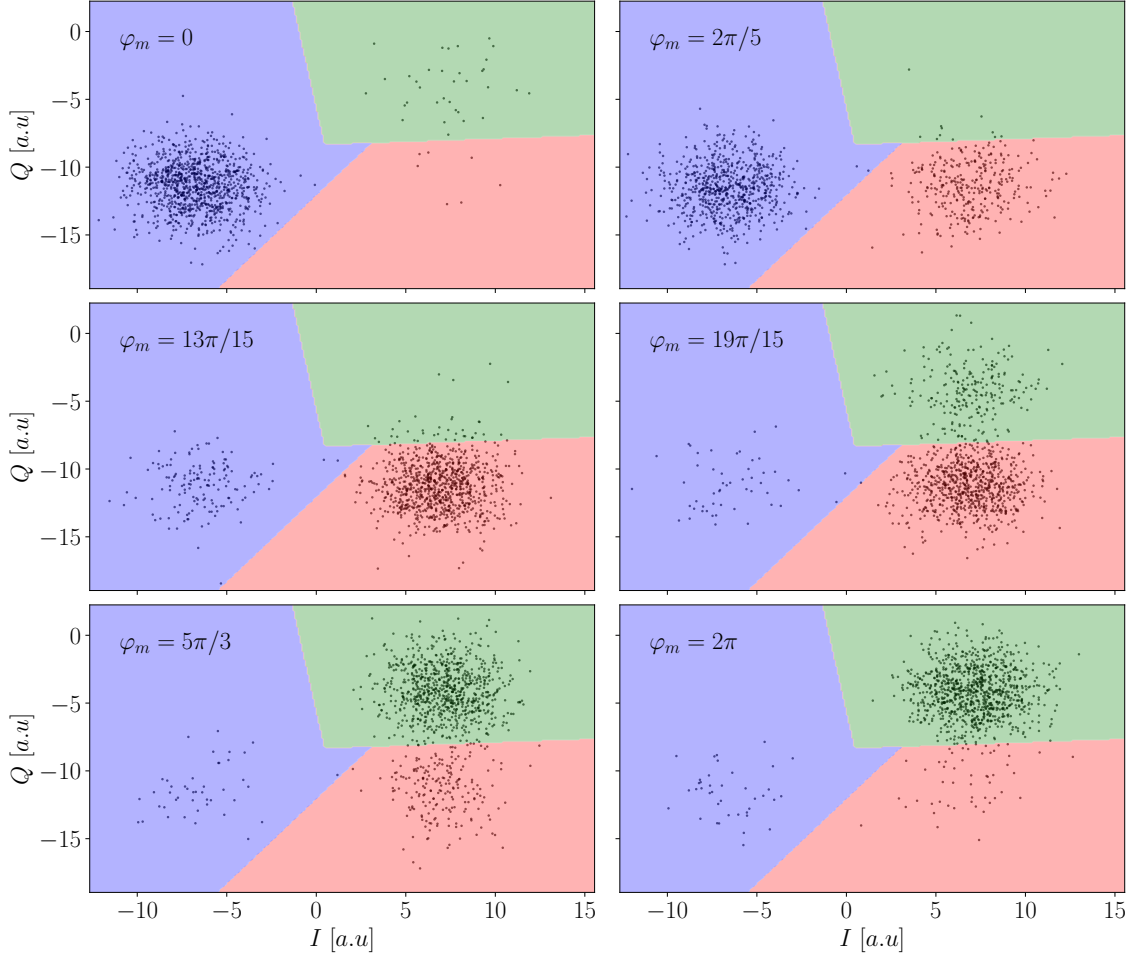


Figure A.2: Example of data distribution associated to the sequential charging protocol. Each plot shows the results (black dots) in the (I, Q) plane (in arbitrary units) as a function of φ_m . For each state shown in the plot, we have considered 1024 runs. These measurements have been carried out using the *ibm_auckland* device. The background is coloured according to what discussed in the calibration phase. In particular the blue part is classified as $|0\rangle$, the red one as $|1\rangle$ and the green one as $|2\rangle$.

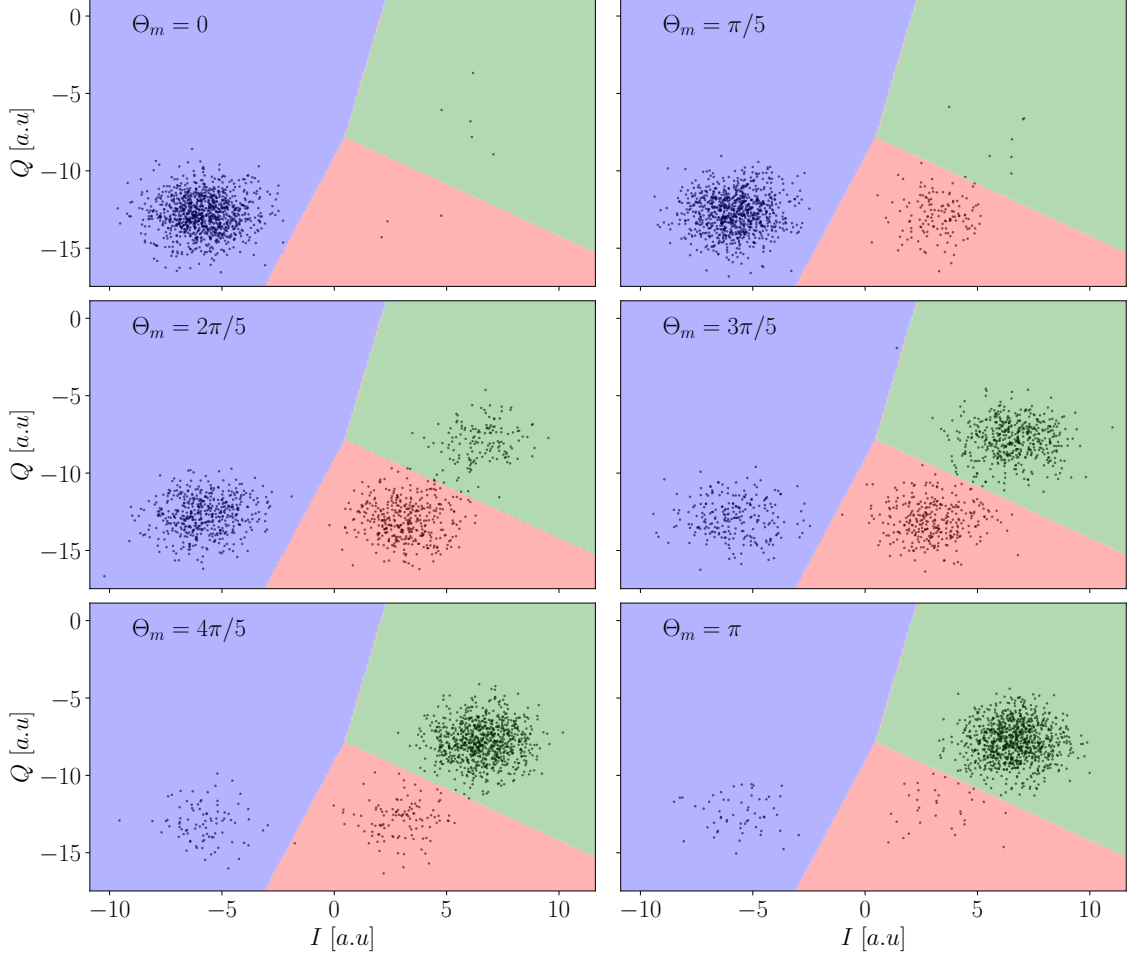


Figure A.3: Example of data distribution associated to the simultaneous charging protocol. Each plot shows the results (black dots) in the (I, Q) plane (in arbitrary units) as a function of Θ_m . For each state shown in the plot, we have considered 1024 runs. These measurements have been carried out using the *ibmq_toronto* device. The background is coloured according to what discussed in the calibration phase. In particular the blue part is classified as $|0\rangle$, the red one as $|1\rangle$ and the green one as $|2\rangle$.

Appendix B

Complements to the Dicke QB in the Off-resonant regime

B.1 Derivation of the Effective LMG Hamiltonian

The aim of this Appendix is to show how it is possible to properly approximate the Dicke Hamiltonian in Eq. (2.94) into the LMG Hamiltonian in Eq. (2.98).

B.1.1 Basics of the Schrieffer–Wolff transformation

Given a generic Hamiltonian $\hat{\mathcal{H}}$ and an operator $\hat{\mathcal{S}}$ it is possible to define [124]

$$\hat{\mathcal{H}}' = e^{\hat{\mathcal{S}}} \hat{\mathcal{H}} e^{-\hat{\mathcal{S}}}. \quad (\text{B.1})$$

According to the Baker-Campbell-Hausdorff relation, we can develop the exponential operators in such a way that

$$\hat{\mathcal{H}}' = \hat{\mathcal{H}} + [\hat{\mathcal{S}}, \hat{\mathcal{H}}] + \frac{1}{2!} [\hat{\mathcal{S}}, [\hat{\mathcal{S}}, \hat{\mathcal{H}}]] + \dots \quad (\text{B.2})$$

On a general ground, it is also possible to assume that $\hat{\mathcal{H}}$ is given by the sum of two terms, namely a free and an interacting term

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{V}}. \quad (\text{B.3})$$

By properly choosing the operator $\hat{\mathcal{S}}$ in such a way to satisfy

$$[\hat{\mathcal{H}}_0, \hat{\mathcal{S}}] = \hat{\mathcal{V}} \quad (\text{B.4})$$

we obtain

$$\hat{\mathcal{H}}' = \hat{\mathcal{H}}_0 + \frac{1}{2} [\hat{\mathcal{S}}, \hat{\mathcal{V}}] + \frac{1}{2} [\hat{\mathcal{S}}, [\hat{\mathcal{S}}, \hat{\mathcal{V}}]] + \dots \quad (\text{B.5})$$

Assuming now that both $\hat{\mathcal{S}}$ and $\hat{\mathcal{V}}$ depend linearly on a given coupling constant, we can consider a second order expansion leading to an effective Hamiltonian of the form

$$\hat{\mathcal{H}}_{\text{eff}} = \hat{\mathcal{H}}_0 + \frac{1}{2} [\hat{\mathcal{S}}, \hat{\mathcal{V}}]. \quad (\text{B.6})$$

In the following, we will apply this general scheme to the Dicke model assuming both single- and two-photon interaction.

B.1.2 Dicke model with single-photon coupling

In the case of the Dicke model with conventional dipole matter-radiation coupling [124, 128] in Eq. (2.94) we can identify

$$\hat{\mathcal{H}}_0 = \omega_z \hat{J}_z + \omega_c \hat{a}^\dagger \hat{a}, \quad (\text{B.7})$$

$$\hat{\mathcal{V}} = 2\lambda \hat{J}_x (\hat{a}^\dagger + \hat{a}), \quad (\text{B.8})$$

and, consequently

$$\hat{\mathcal{S}} = \frac{\lambda}{\omega_c - \omega_z} [\hat{J}_- \hat{a}^\dagger - \hat{J}_+ \hat{a}] + \frac{\lambda}{\omega_c + \omega_z} [\hat{J}_+ \hat{a}^\dagger - \hat{J}_- \hat{a}], \quad (\text{B.9})$$

with

$$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y. \quad (\text{B.10})$$

Notice that both Eq. (B.8) and (B.9) are linear in the matter-radiation coupling λ as required by the previous discussion. Using the Schrieffer–Wolff transformation discussed above we obtain the effective Hamiltonian

$$\hat{\mathcal{H}}_{\text{eff}} = \omega_z \hat{J}_z + \omega_c \hat{a}^\dagger \hat{a} - \frac{2\lambda^2 \omega_z}{\omega_c^2 - \omega_z^2} \hat{J}_z (\hat{a}^\dagger + \hat{a})^2 - \frac{4\lambda^2 \omega_c}{\omega_c^2 - \omega_z^2} \hat{J}_x^2, \quad (\text{B.11})$$

which is a good approximation of the Dicke Hamiltonian in the so called dispersive regime $\lambda_0 \ll |\omega_c - \omega_z|$ [124]. Notice that, in this regime, the possibility to increase the energy stored into a QB through virtual excitations mediated by a higher excited state has been also discussed in Ref. [220]. Further considering the limit $\omega_c \gg \omega_z$ we finally have

$$\hat{\mathcal{H}}_D^{(O)} = \omega_z \hat{J}_z + \omega_c \hat{a}^\dagger \hat{a} - \frac{4\lambda^2}{\omega_c} \hat{J}_x^2 \quad (\text{B.12})$$

that is Eq. (2.98) in the main text.

Getting rid of the cavity contribution it is possible to map Eq. (B.12) into

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_B + \hat{\mathcal{H}}_{\text{int}} \quad (\text{B.13})$$

$$= \omega_z \hat{J}_z - g \hat{J}_x^2, \quad (\text{B.14})$$

with

$$g = \frac{4\lambda^2}{\omega_c}. \quad (\text{B.15})$$

Notice that, according to this mapping, only positive values of the parameter g are physically meaningful. Moreover, as shown in the following Section, even a more exotic two-photon matter-radiation coupling [221, 222] leads to an analogous effective Hamiltonian.

B.1.3 Dicke model with two-photon coupling

This more exotic interaction can be obtained by properly engineering both atomic and solid state systems [221, 222]. Here, we can write the Hamiltonian

$$\hat{\mathcal{H}}_{\text{Dicke}}^{2ph} = \omega_z \hat{J}_z + \omega_c \hat{a}^\dagger \hat{a} + 2\lambda \hat{J}_x \left[(\hat{a}^\dagger)^2 + (\hat{a})^2 \right], \quad (\text{B.16})$$

identifying

$$\hat{\mathcal{H}}_0 = \omega_z \hat{J}_z + \frac{\omega_c}{2} \hat{a}^\dagger \hat{a}, \quad (\text{B.17})$$

$$\hat{\mathcal{V}} = 2\lambda \hat{J}_x \left[(\hat{a}^\dagger)^2 + \hat{a}^2 \right], \quad (\text{B.18})$$

and consequently

$$\hat{\mathcal{S}} = \frac{\lambda}{\omega_c - \omega_z} \left[\hat{J}_- (\hat{a}^\dagger)^2 - \hat{J}_+ \hat{a}^2 \right] + \frac{\lambda}{\omega_c + \omega_z} \left[\hat{J}_+ (\hat{a}^\dagger)^2 - \hat{J}_- \hat{a}^2 \right]. \quad (\text{B.19})$$

According to the previous analysis, we obtain the effective Hamiltonian

$$\hat{\mathcal{H}}_{\text{eff}}^{2ph} = \omega_z \hat{J}_z + \frac{\omega_c}{2} \hat{a}^\dagger \hat{a} - \frac{2\lambda^2 \omega_z}{\omega_c^2 - \omega_z^2} \hat{J}_z \left[\hat{a}^2 + (\hat{a}^\dagger)^2 \right]^2 - \frac{4\lambda^2 \omega_c}{\omega_c^2 - \omega_z^2} \hat{J}_x^2 (\hat{a} \hat{a}^\dagger + \hat{a}^\dagger \hat{a}), \quad (\text{B.20})$$

which again represents a good approximation of the two-photon Dicke Hamiltonian in the dispersive limit $\lambda \ll |\omega_c - \omega_z|$.

Further considering the limit $\omega_c \gg \omega_z$ we finally have

$$\hat{\mathcal{H}}_{\text{eff}}'^{2ph} = \omega_z \hat{J}_z + \frac{\omega_c}{2} \hat{a}^\dagger \hat{a} - \frac{4\lambda^2}{\omega_c} (2\hat{a}^\dagger \hat{a} + 1) \hat{J}_x^2. \quad (\text{B.21})$$

For proper initial states of the photon in the cavity, it is possible to map Eq. (B.21) into Eq. (B.14) (up to a constant) by defining

$$g = \frac{4\lambda^2}{\omega_c} (2n + 1), \quad (\text{B.22})$$

with n the averaged number of photons into the cavity. Notice that in this case the renormalization of the effective coupling due to the presence of the cavity photons can be exploited to increase the value of g with respect to the previous case.

B.2 Comments on the classical limit

In the main text, we have considered the scaling at a finite number of TLSs, without addressing the thermodynamical limit needed for a proper study of the ESQPT. Some hints in this direction can be derived starting from the classical version of the Hamiltonian in Eq. (2.94). This can be obtained replacing the operators $\hat{J}_{x,y,z}$ with the classical angular momentum components

$$J_x = \frac{N}{2} \sin \theta \cos \varphi, \quad (\text{B.23})$$

$$J_y = \frac{N}{2} \sin \theta \sin \varphi, \quad (\text{B.24})$$

$$J_z = \frac{N}{2} \cos \theta. \quad (\text{B.25})$$

This leads to the classical Hamiltonian

$$H_{\text{cl}} = \omega_z \frac{N}{2} \cos \theta - g \frac{N^2}{4} \sin^2 \theta \cos^2 \varphi. \quad (\text{B.26})$$

One can identify now two conjugated variables [223]

$$q = N \cos \theta, \quad (\text{B.27})$$

$$p = \varphi, \quad (\text{B.28})$$

in such a way that

$$H_{\text{cl}} = \frac{\omega_z}{2} q - \frac{g}{4} N^2 \cos^2 p + \frac{g}{4} q^2 \cos^2 p. \quad (\text{B.29})$$

Recalling the equations of motion

$$\frac{dq}{dt} = \frac{\partial H_{\text{cl}}}{\partial p} = \frac{g}{4} N^2 \sin 2p - \frac{g}{4} q^2 \sin 2p, \quad (\text{B.30})$$

$$\frac{dp}{dt} = -\frac{\partial H_{\text{cl}}}{\partial q} = -\frac{\omega_z}{2} + \frac{g}{2} q \cos^2 p. \quad (\text{B.31})$$

Further manipulating the above Equations introducing rescaled and shifted variables

$$q = N \tilde{q}, \quad (\text{B.32})$$

$$p = \tilde{p} - \frac{\omega_z}{2} t, \quad (\text{B.33})$$

one has

$$\frac{d\tilde{q}}{dt} = \frac{g}{4} N (1 - \tilde{q}^2) \sin (2\tilde{p} - \omega_z t), \quad (\text{B.34})$$

$$\frac{d\tilde{p}}{dt} = -\frac{g}{2} N \tilde{q} \cos^2 \left(\tilde{p} - \frac{\omega_z}{2} t \right), \quad (\text{B.35})$$

where clearly emerge the dependence on the renormalized interaction parameter

$$G = gN \quad (\text{B.36})$$

which plays a major role in the discussion about the universality reported in the main text.

B.3 Perturbative Approach to the Weak Coupling Regime

In the weak coupling regime, it is possible to study the dynamics induced by Eq. (B.14) and the figures of merits discussed in the main text by applying the time-dependent perturbation theory in terms of the Dyson series.

Working in the Interaction picture (indicated in the following by the apex I), the time evolution operator $\hat{U}_I(t, 0)$ from the initial time $t = 0$ to a generic time t satisfies the differential equation

$$i\partial_t \hat{U}_I(t, 0) = \hat{\mathcal{H}}_{\text{int}}^I(t) \hat{U}_I(t, 0), \quad (\text{B.37})$$

with

$$\begin{aligned} \hat{\mathcal{H}}_{\text{int}}^I(t) &= -g e^{i\omega_z t \hat{J}_z} \hat{J}_x^2 e^{-i\omega_z t \hat{J}_z} \\ &= -g e^{i\omega_z t \hat{J}_z} \hat{J}_x e^{-i\omega_z t \hat{J}_z} e^{i\omega_z t \hat{J}_z} \hat{J}_x e^{-i\omega_z t \hat{J}_z} \\ &= -g [\cos(\omega_z t) \hat{J}_x^2 - \sin(\omega_z t) \cos(\omega_z t) (\hat{J}_x \hat{J}_y + \hat{J}_y \hat{J}_x) + \\ &\quad + \sin(\omega_z t) \hat{J}_y^2]. \end{aligned} \quad (\text{B.38})$$

Imposing the initial condition $\hat{U}_I(0, 0) = 1$ and formally integrating the above equation we have

$$\hat{U}_I(t, 0) = 1 - i \int_0^t \hat{\mathcal{H}}_{\text{int}}^I(t') \hat{U}_I(t', 0) dt'. \quad (\text{B.39})$$

We can solve iteratively this equation in terms of Dyson's series [50]

$$\hat{U}_I(t, 0) = 1 - i \int_0^t \hat{\mathcal{H}}_{\text{int}}^I(t') dt' + (-i)^2 \int_0^t dt' \int_0^{t'} dt'' \hat{\mathcal{H}}_{\text{int}}^I(t') \hat{\mathcal{H}}_{\text{int}}^I(t'') + \dots \quad (\text{B.40})$$

In this picture, the energy stored in the QB can be written as

$$\begin{aligned} E_B(t) &= \left\langle \frac{N}{2}, -\frac{N}{2} \left| e^{-i\hat{\mathcal{H}}_0 t} \hat{U}_I^\dagger(t, 0) \hat{\mathcal{H}}_B \hat{U}_I(t, 0) e^{i\hat{\mathcal{H}}_0 t} \right| \frac{N}{2}, -\frac{N}{2} \right\rangle \\ &= \left\langle \frac{N}{2}, -\frac{N}{2} \left| \hat{\mathcal{H}}_B \right| \frac{N}{2}, -\frac{N}{2} \right\rangle \\ &= \left\langle \frac{N}{2}, -\frac{N}{2} \left| \hat{U}_I^\dagger(t, 0) \hat{\mathcal{H}}_B \hat{U}_I(t, 0) \right| \frac{N}{2}, -\frac{N}{2} \right\rangle + \frac{\omega_z}{2} N. \end{aligned} \quad (\text{B.41})$$

After some long and tedious algebra, we finally obtain

$$E_B^{(w)}(t) = \frac{g^2}{8} \frac{1 - \cos 2\omega_z t}{\omega_z} (N^2 - N), \quad (\text{B.42})$$

and consequently

$$P^{(w)}(t) = \frac{E(t)}{t} = \frac{g^2}{8} \frac{1 - \cos 2\omega_z t}{t\omega_z} (N^2 - N). \quad (\text{B.43})$$

Appendix C

Complements to Chapter 3

C.1 Minimal model of cyclic bipartite quantum battery

In this Appendix, we introduce an example of quantum circuit described by the model presented in Chapter 3. We consider a setup based on three symmetrical dc-SQUIDs, see Fig. C.1, originally proposed in [224] as quantum storage unit and later as a possible experimental setup for a Maxwell's demon-assisted quantum heat engine [225].

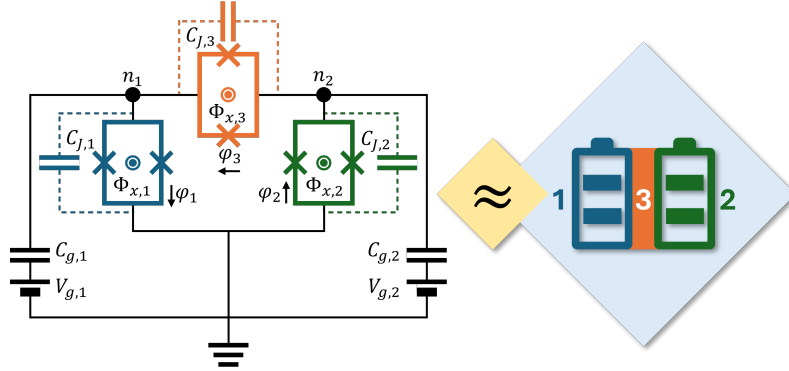


Figure C.1: Schematic circuit of the proposed Josephson QB based on three dc-SQUIDs pierced by externally tunable magnetic fluxes. Josephson junctions are denoted by a cross and the black circles, labelled by n_1 and n_2 , correspond to the first and second Cooper pair box, respectively. The three dc-SQUIDs operate under the qubit approximation. The qubit 3, used as a quantum coupler, mediates an effective interaction between qubits 1 and 2. For the present setup to be used as a cyclic quantum battery we set $C_{J,3} = 0$, so that $E_3 = 0$ in Eq. (C.1). Removing the flux-independent interaction between qubits 1 and 2 allows them to be fully disconnected by the externally-driven magnetic flux. Image taken from [22].

The Hamiltonian of the system comprises charging and Josephson energy contribution. When the Josephson energy is much weaker than the charging energy, the evolution is approximately confined into the two-dimensional space spanned by the eigenstates of the charge operator, $\{|0\rangle_k, |1\rangle_k\}$ of the k -th Cooper pair box ($k = 1, 2, 3$), introduced in Section 1.2.3. Under this condition and the constraint $\varphi_1 + \varphi_2 + \varphi_3 = 0$ on the phase differences φ_k in the k -th dc-SQUID, it is possible to

derive an effective (pseudo)-spin Hamiltonian of the form

$$\begin{aligned}\hat{\mathcal{H}} &= \sum_{k=1}^2 \Omega_k \hat{\sigma}_k^z + E_3 \hat{\sigma}_1^z \hat{\sigma}_2^z - \sum_{k=1}^2 E_{J,k} \cos \left(\pi \frac{\Phi_{x,k}}{\Phi_0} \right) \hat{\sigma}_k^x \\ &- E_{J,3} \cos \left(\pi \frac{\Phi_{x,3}}{\Phi_0} \right) (\hat{\sigma}_1^x \hat{\sigma}_2^x - \hat{\sigma}_1^y \hat{\sigma}_2^y).\end{aligned}\quad (\text{C.1})$$

In this setup, the bipartite QB comprises the first two dc-SQUIDs, while the third one plays the role of a tunable quantum coupler between them [130–132]. In the Hamiltonian in Eq. (C.1), $E_{J,k}$ and $\Phi_{x,k}$ are, respectively, the Josephson energy and the magnetic flux in the k -th dc-SQUID, while $\Phi_0 = h/2e$ is the superconducting flux quantum, with h the Planck constant and e the elementary charge. Moreover, $\Omega_k = E_{C,k}(n_{g,k} - 1/2) + 2E_3(n_{g,j} - 1/2)$, with $j \neq k$, where $n_{g,k} = C_{g,k}V_{g,k}/2e$, with $V_{g,k}$ and $C_{g,k}$ being respectively the gate voltage and capacitance in the k -th Cooper pair box. The other coefficients are $E_{C,k} = 2e^2 C_{\Sigma,j} / (C_{\Sigma,1}C_{\Sigma,2} - C_{J,3}^2)$, with $j \neq k$, and $E_3 = e^2 C_{J,3}/2 (C_{\Sigma,1}C_{\Sigma,2} - C_{J,3}^2)$, with $C_{\Sigma,k} = C_{J,k} + C_{J,3} + C_{g,k}$.

One of the key advantages of the proposed basic scheme (Fig. C.1), which relies on dc-SQUID charge qubits [226, 227] designed to operate in the regime $k_B T \ll E_C$ [228] and $E_C \gg E_J$, is its experimental feasibility. Therefore, we now examine experimentally feasible parameters considering comparable platforms and setups. Suitable values of the junction capacitance are in the range of femtofarad and below, $C_{J,k} \leq 1$ fF, while the gate capacitances $C_{g,k}$ can be even smaller [229] (e.g., $C_{g,k} \sim 0.6$ aF and $C_{J,k} \sim 620$ aF [230]). The dimensionless gate charge usually takes values $n_{g,k} \sim 0 \div 2$ [231, 232]. Charging energies $E_{C,k}/h \sim 10 \div 100$ GHz [230] and Josephson energies $E_{J,k}/h \sim 1 \div 10$ GHz fulfilling the condition $E_C \gg E_J$ are consistent with experimental setups [230]. Regarding the dc-SQUID geometry, an effective area can be estimated in $A \approx 4.9 \mu\text{m}^2$ which, provided a magnetic field $B_x \sim 0.1 \div 1$ mT, results in a magnetic flux threading the dc-SQUID loop $\Phi_x/\Phi_0 = B_x A/\Phi_0 \sim 0.237 \div 2.37$, with $\Phi_0 = 2.067$ fWb [233]. Assuming $n_{g,k} = 1$ ¹ and $C_{g,k} = 2$ aF, we can estimate the gate voltage $V_{g,k} = 2en_{g,k}/C_{g,k} \approx 160$ mV. Finally, a typical temperature is $T \sim 30$ mK ($k_B T/h \sim 0.625$ GHz) [227].

Based on the dc-SQUIDs setup just described, we can consider the following Hamiltonian

$$\hat{\mathcal{H}} = \Omega \sum_{k=1}^2 \hat{\sigma}_k^z - E_J \cos \left(\pi \frac{\Phi_x}{\Phi_0} \right) \left[\sum_{k=1}^2 \hat{\sigma}_k^x + (\hat{\sigma}_1^x \hat{\sigma}_2^x - \hat{\sigma}_1^y \hat{\sigma}_2^y) \right], \quad (\text{C.2})$$

obtained from Eq. (C.1) under the assumptions: $E_3 = 0$; $\Phi_{x,k} = \Phi_x$ and $E_{J,k} = E_J$ for $k = 1, 2, 3$; $E_{C,k} = E_C$ and $n_{g,k} = n_g$, from which $\Omega_k = \Omega = E_C(n_g - 1/2)$, for $k = 1, 2$. In addition, the two-level approximation requires $E_C \gg E_J$. The assumption of equal magnetic fluxes Φ_x is motivated by the will of reducing the number of free parameters, together with the fact that, considering dc-SQUIDs with the same loop geometry, it is experimentally easier to have an approximately homogeneous magnetic field piercing the three Cooper pair boxes, instead of strong inhomogeneities at nanoscale [234]. Letting $\Phi_x = \Phi_x(t)$, the magnetic flux can be regarded to as the external driving which modulates the interaction $\hat{\sigma}_1^x \hat{\sigma}_2^x - \hat{\sigma}_1^y \hat{\sigma}_2^y$, in particular, switches it on or off, but also the single-qubit contributions $\propto \hat{\sigma}_k^x$, a

¹For later convenience, we require $n_{g,k} = n_g > 1/2$ to ensure $\Omega_k = \Omega > 0$ in Eq. (C.2).

side effect specific of the model from which we derived the Hamiltonian. Switching on/off the interaction, however, in general does not suffice to fully disconnect the two qubits, because of the residual interaction $\propto \hat{\sigma}_1^z \hat{\sigma}_2^z$, independent of the magnetic flux (see Eq. (C.1)). The assumption $E_3 = 0$, accomplished by setting $C_{J,3} = 0$, allows us to discard the interaction $\propto \hat{\sigma}_1^z \hat{\sigma}_2^z$ fully disconnecting qubits through the magnetic flux.

Considering Ω as the reference scale for the energies, we can further simplify the Hamiltonian in Eq. C.2 into

$$\begin{aligned}\hat{\mathcal{H}}(t) &= \hat{\sigma}_A^z + \hat{\sigma}_B^z - \gamma(t)(\hat{\sigma}_A^x + \hat{\sigma}_B^x + \hat{\sigma}_A^x \hat{\sigma}_B^x - \hat{\sigma}_A^y \hat{\sigma}_B^y) \\ &\equiv \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{int}}(t),\end{aligned}\tag{C.3}$$

where, we have identified the bare Hamiltonian, $\hat{\mathcal{H}}_0$, and the driven one, $\hat{\mathcal{H}}_{\text{int}}(t)$ with $\gamma(t) = \theta(\bar{t} - t)\gamma_0$ with $\gamma_0 \neq 0$. Notice that $\hat{\mathcal{H}}_{\text{int}}(t)$ includes single-qubit terms, in addition to the two-qubit interaction. (Dis)connecting the two qubits is related to switching on (off) $\hat{\mathcal{H}}_{\text{int}}$. In the dc-SQUIDS system, after identifying $\gamma(t) \equiv E_J \cos(\pi\Phi_x(t)/\Phi_0)/\Omega$, this is accomplished by tuning the magnetic flux to $\Phi_x^{(\text{off})} = (m + 1/2)\Phi_0$, with $m \in \mathbb{Z}$, for full disconnection ($\gamma(t) = 0$) and to any other value, $\Phi_x^{(\text{on})} \neq \Phi_x^{(\text{off})}$, for a connection at arbitrary coupling strength ($\gamma(t) = \gamma_0 \equiv E_J \cos(\pi\Phi_x^{(\text{on})}/\Phi_0)/\Omega$). Therefore, for a given configuration of the setup, γ_0 can be externally tuned through the magnetic flux without changing the circuit elements and can take negative values depending on the value of the cosine function. Its possible values are limited to $|\gamma_0| \ll (n_g - 1/2)^{-1}$ due to the condition $E_C \gg E_J$.

C.1.1 Possible experimental scenario

Finally, we elaborate on admissible configurations of the specific superconducting setup discussed in the previous Section in relation to our assumptions and to the results discussed in Section 3.3.

First, we provide a possible estimate of the timescale over which ergotropy is extracted from the single qubit in the s -JQB. The unitary operation in Eq. (2.27) which accomplishes this task is the product of two rotations $R_a(\phi) = e^{i\phi\hat{\sigma}_a/2}$, with $a = x, y, z$, one about the y -axis (responsible for extracting ergotropy) and one about the z -axis (which does not affect the ergotropy). Therefore, assuming $\theta = 0$, we can ultimately focus on $R_y(2\alpha)$, which can be decomposed in terms of rotations only about the x - and z -axis, $R_y(2\alpha) = R_z(3\pi)R_x(\pi/2)R_z(\pi + 2\alpha)R_x(\pi/2)$, each of which can be realized using finite duration voltage bias pulses [235], with corresponding frequencies $\nu_x = E_J/h$ and $\nu_z = E_C(n_g - 1/2)/h$. Considering pulses of duration of the order ~ 100 ps, to account for possible experimental constraints on the shortest duration of a pulse [236], we can estimate the timescale of extraction of ergotropy as ~ 1 ns, much shorter than the typical longitudinal and transverse relaxation times of superconducting charge qubits $T_1 \sim 1 \div 10 \mu\text{s}$ and $T_2 \sim 0.1 \div 1 \mu\text{s}$ [237], respectively. Since thermalization involves relaxation processes, our assumption that the only role played by the reservoir is to thermalize the system at the end of every cycle is consistent with the time scales estimated above. This assumption works when the temperature is sufficiently low. For the superconducting setup introduced above, this is the case when $k_B T \ll E_C$, being a typical temperature $k_B T/h \sim 0.625$ GHz [227] and $E_C/h \sim 10 \div 100$ GHz. In this regard, we want to

stress that the results in Fig. 3.2, and in the following, are expressed in units of $\Omega = E_C (n_g - 1/2)$. Therefore, the fact that Ω depends also on the dimensionless gate charge n_g , whose value can be tuned through the gate voltage of the Cooper pair boxes [231], allows for investigating regimes not limited to $k_B T \ll \Omega$, while keeping $k_B T \ll E_C$ (the low temperature regime).

A possible experimental scenario consistent with Fig. 3.2(a) at fixed $T = 0.5\Omega/k_B = 30$ mK [227] is obtained for $C_J = 900$ aF, $C_g = 1.65$ aF, $V_g = 100$ mV, resulting in $n_g \approx 0.515$, $E_C/h \approx 86$ GHz and $\Omega/h = 1.28$ GHz. These values, for $E_J/h \sim 10$ GHz, allow to explore the range $|\gamma_0| \leq 7.8$ while fulfilling $E_J, k_B T \ll E_C$. On the other hand, the same set of parameters provides $\gamma_0 \approx 0.78$ for $E_J/h \approx 1$ GHz, consistently with $\gamma_0 = 0.8$ in Fig. 3.2(b), where $T \leq 10\Omega$ still fulfills $k_B T \ll E_C$.

C.2 Details on the energetics of the working cycle of the JQB

In this Appendix, we provide the analytical derivation of the results presented in Section 3.2, regarding the energetics of the p -JQB for the different Protocols (i)–(iii), $p = s, l, g$, respectively. First, we focus on the energetics of the protocols $p = s, l$, in which ergotropy is locally extracted from qubits. We then address the energetics of the protocol $p = g$, which requires an extended discussion due to the presence of a degenerate energy level in the bare Hamiltonian $\hat{\mathcal{H}}_0 = \hat{\mathcal{H}}_A + \hat{\mathcal{H}}_B$, from which the global ergotropy is extracted.

We observe that $\langle \hat{\sigma}_A^i \rangle = \langle \hat{\sigma}_B^i \rangle$ and $\langle \hat{\sigma}_A^i \hat{\sigma}_B^j \rangle = \langle \hat{\sigma}_A^j \hat{\sigma}_B^i \rangle$ with $i, j = x, y, z$, since the Hamiltonian in Eq. (3.11), hence the Gibbs state, is symmetric under exchange of the two qubits. Accordingly, the results that follow will be expressed in terms of $\langle \hat{\sigma}_A^i \rangle$ and $\langle \hat{\sigma}_A^i \hat{\sigma}_B^j \rangle$.

C.2.1 Energetics of the ($p = s, l$)-JQB

The connection energy in Eq. (3.3) for the s -JQB reads (identifying $\hat{U}_A(\theta_A) \equiv \hat{U}(\theta)$ for notational convenience)

$$E_c^{(s)}(\theta) = -\gamma_0 (\langle \hat{U}^\dagger(\theta) \hat{\sigma}_A^x \hat{U}(\theta) \rangle + \langle \hat{\sigma}_B^x \rangle + \langle \hat{U}^\dagger(\theta) \hat{\sigma}_A^x \hat{U}(\theta) \otimes \hat{\sigma}_B^x \rangle - \langle \hat{U}^\dagger(\theta) \hat{\sigma}_A^y \hat{U}(\theta) \otimes \hat{\sigma}_B^y \rangle), \quad (\text{C.4})$$

where the cyclic property of the trace has been used. Therefore, we have to compute $\hat{U}^\dagger(\theta) \hat{\sigma}_A^a \hat{U}(\theta)$, with $a = x, y$ and $\hat{U}(\theta)$ in Eq. (2.27). By direct inspection it is possible to prove that

$$\hat{U}^\dagger(\theta) \hat{\sigma}_A^x \hat{U}(\theta) = \cos(2\theta) \cos(2\alpha) \hat{\sigma}_A^x + \sin(2\theta) \hat{\sigma}_A^y - \cos(2\theta) \sin(2\alpha) \hat{\sigma}_A^z, \quad (\text{C.5})$$

$$\hat{U}^\dagger(\theta) \hat{\sigma}_A^y \hat{U}(\theta) = -\sin(2\theta) \cos(2\alpha) \hat{\sigma}_A^x + \cos(2\theta) \hat{\sigma}_A^y + \sin(2\theta) \sin(2\alpha) \hat{\sigma}_A^z. \quad (\text{C.6})$$

For a real state ϱ_I (as a Gibbs state is), $\langle \hat{\sigma}_A^y \rangle = \langle \hat{\sigma}_A^y \hat{\sigma}_B^x \rangle = \langle \hat{\sigma}_A^y \hat{\sigma}_B^z \rangle = 0$. Combining all previous results, Eq. (3.15) follows.

Analogously, we can compute the connection energy for the l -JQB, recalling that

the two-qubit unitary is $\hat{\mathcal{U}}_l(\theta_A, \theta_B) = \hat{U}_A(\theta_A) \otimes \hat{U}_B(\theta_B)$ with $\hat{U}_k(\theta_k)$ in Eq. (2.27),

$$\begin{aligned} E_c^{(l)}(\theta_A, \theta_B) = & - \gamma_0 \left\{ \left(\cos(2\theta_A) + \cos(2\theta_B) \right) \left(\cos(2\alpha) \langle \hat{\sigma}_A^x \rangle \right. \right. \\ & - \left. \sin(2\alpha) \langle \hat{\sigma}_A^z \rangle \right) + \cos[2(\theta_A + \theta_B)] \left(\cos^2(2\alpha) \langle \hat{\sigma}_A^x \hat{\sigma}_B^x \rangle \right. \\ & - \left. \langle \hat{\sigma}_A^y \hat{\sigma}_B^y \rangle + \sin^2(2\alpha) \langle \hat{\sigma}_A^z \hat{\sigma}_B^z \rangle - \sin(4\alpha) \langle \hat{\sigma}_A^x \hat{\sigma}_B^z \rangle \right) \Big\}. \end{aligned} \quad (\text{C.7})$$

Note that, in principle, such a unitary depends on two independent arbitrary phases. Now, we observe that $\cos(2\alpha) \langle \hat{\sigma}_A^x \rangle - \sin(2\alpha) \langle \hat{\sigma}_A^z \rangle = 0$, and, provided that $\alpha \neq \frac{\pi}{2} + k\pi$ with $k \in \mathbb{Z}$,

$$\begin{aligned} \cos(2\alpha) &= \frac{1 - \tan^2 \alpha}{1 + \tan^2 \alpha} = -\frac{z}{r}, \\ \sin(2\alpha) &= \frac{2 \tan \alpha}{1 + \tan^2 \alpha} = -\frac{x}{r}, \end{aligned} \quad (\text{C.8})$$

because $\alpha = \arctan[-(r+z)/x]$ with $y = 0$. Therefore, $E_c^{(l)}(\theta_A, \theta_B) = E_c^{(l)}(\theta_A + \theta_B)$ is a function of a single effective parameter. This concludes the proof of Eq. (3.16).

C.2.2 Energetics of the g -JQB

In the g -JQB, the resource for extracting work comprises both the subsystems and the correlations. The state from which the global ergotropy $\mathcal{E}^{(g)}$ is extracted is the thermal state $\varrho_{\text{II}} = \varrho_{\text{I}} = \tau_\beta$ with Hamiltonian $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{int}}$ in Eq. (3.11). The purpose of this protocol is to extract $\mathcal{E}^{(g)}$ with respect to the bare Hamiltonian $\hat{\mathcal{H}}_0 = \hat{\sigma}_A^z + \hat{\sigma}_B^z$. Indeed, τ_β is passive with respect to $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{int}}$ but can be active with respect to $\hat{\mathcal{H}}_0$. Therefore, disconnecting the qubits is still a necessary condition for the working cycle based on this protocol. When ergotropy is globally extracted from a system, the passive state is not unique if there are degeneracies in the energy spectrum [60].

In the present case, ergotropy is extracted from τ_β with respect to $\hat{\mathcal{H}}_0$. The two eigenstates associated with the degenerate zero-energy level are $|01\rangle$ and $|10\rangle$. The presence of a degenerate eigenvalue makes the eigendecomposition of $\hat{\mathcal{H}}_0$ not unique, which, in turn, results in ambiguity in the definition of the unitary $\hat{\mathcal{U}}_g$ in Eq. (2.17) by means of which one would like to extract the global ergotropy $\mathcal{E}^{(g)}$. Below, we show that this ambiguity does not affect the global ergotropy $\mathcal{E}^{(g)}$ and that, in the present model (g -JQB), $E_c^{(g)} \equiv 0$.

The aforementioned arbitrariness can be encoded in a unitary operator $\hat{u}$, such that $[\hat{\mathcal{H}}_0, \hat{u}] = 0$, which effectively acts only on the degenerate subspace of $\hat{\mathcal{H}}_0$ spanned by $\{|01\rangle, |10\rangle\}$, and so that $\hat{u}|00\rangle = |00\rangle$ and $\hat{u}|11\rangle = |11\rangle$. In the computational basis, this operator can be represented by

$$\hat{u} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & u_{01,01} & u_{01,10} & 0 \\ 0 & u_{10,01} & u_{10,10} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad (\text{C.9})$$

with $\hat{u}\hat{u}^\dagger = \hat{u}^\dagger\hat{u} = \hat{I}$. Accordingly, we introduce the unitary (see Eq. (2.17))

$$\hat{\mathcal{U}}_{g;\hat{u}} = \hat{u} \sum_{k=1}^4 |\epsilon_k^{(0)}\rangle \langle \lambda_k| \equiv \hat{u} \hat{\mathcal{U}}_g, \quad (\text{C.10})$$

where the eigenstates of $\hat{\mathcal{H}}_0$, $\{|\epsilon_k^{(0)}\rangle\}_k$ with associated eigenvalues $\{\epsilon_k^{(0)}\} = \{-2, 0, 0, 2\}$, are the computational basis states sorted in reverse order (from the lowest energy state $|\epsilon_1^{(0)}\rangle = |11\rangle$ to the highest one $|\epsilon_4^{(0)}\rangle = |00\rangle$), $\{|\lambda_k\rangle\}_k$ the eigenstates of τ_β . By construction, the unitary operation in Eq. (C.10) is expected to extract the global ergotropy, but its definition depends on $\hat{u}$. Starting from the orthonormal eigenstates $|01\rangle$ and $|10\rangle$, the effective purpose of $\hat{u}$ is to span orthonormal pairs of states - a unitary transformation preserves norm and inner product - from the degenerate subspace associated with $\epsilon_2^{(0)} = \epsilon_3^{(0)} = 0$, without affecting $|00\rangle$ and $|11\rangle$.

The arbitrariness of $\hat{\mathcal{U}}_{g;\hat{u}}$ in Eq. (C.10) results in an ambiguity in the passive state $\pi_{g;\hat{u}} = \hat{u}\pi_g\hat{u}^\dagger$, where $\pi_g = \text{diag}(\lambda_4, \lambda_3, \lambda_2, \lambda_1)$ is the diagonal state obtained by using the identity in place of $\hat{u}$. In the computational basis, the passive state is of the form

$$\pi_{\hat{u}} = \begin{pmatrix} \lambda_4 & 0 & 0 & 0 \\ 0 & (\pi_{\hat{u}})_{01,01} & (\pi_{\hat{u}})_{01,10} & 0 \\ 0 & (\pi_{\hat{u}})_{10,01} & (\pi_{\hat{u}})_{10,10} & 0 \\ 0 & 0 & 0 & \lambda_1 \end{pmatrix}. \quad (\text{C.11})$$

The global ergotropy $\mathcal{E}^{(g)}(\tau_\beta) \equiv \text{Tr}[\hat{\mathcal{H}}_0\tau_\beta] - \text{Tr}[\hat{\mathcal{H}}_0\pi_g]$ turns out to be independent of $\hat{u}$, because $\text{Tr}[\hat{\mathcal{H}}_0\pi_{\hat{u}}] = \text{Tr}[\hat{\mathcal{H}}_0\pi_g]$ since $[\hat{\mathcal{H}}_0, \hat{u}] = 0$. In particular, it reads

$$\mathcal{E}^{(g)} = \text{Tr}[(\hat{\sigma}_A^z + \hat{\sigma}_B^z)\tau_\beta] - \sum_{k=1}^4 \lambda_k \epsilon_k^{(0)} = 2\langle \hat{\sigma}_A^z \rangle - 2(\lambda_4 - \lambda_1), \quad (\text{C.12})$$

where $\lambda_1 = e^{-\beta\epsilon_1}/Z$ and $\lambda_4 = e^{-\beta\epsilon_4}/Z$. In the derivation, we have used $\hat{\mathcal{U}}_g$ in Eq. (C.10), $\hat{\mathcal{H}}_0 = \sum_{k=1}^4 \epsilon_k^{(0)} |\epsilon_k^{(0)}\rangle\langle\epsilon_k^{(0)}|$ with $\{\epsilon_k^{(0)}\} = \{-2, 0, 0, 2\}$, and $\tau_\beta = \sum_{k=1}^4 \lambda_k |\lambda_k\rangle\langle\lambda_k|$, whose eigenvalues $\lambda_k = e^{-\beta\epsilon_k}/Z$ involve the partition function $Z = \text{Tr}[e^{-\beta\hat{\mathcal{H}}}]$ of the Hamiltonian $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \gamma_0\hat{\mathcal{H}}_{\text{int}}$, whose eigenvalues $\{\epsilon_k\}_k$ are given in App. C.2.3. This concludes the proof of $\mathcal{E}^{(g)}$ in Eq. (3.14).

Now, we prove that $E_c^{(g)} = \gamma_0 \text{Tr}[\hat{\mathcal{H}}_{\text{int}}\pi_{\hat{u}}] \equiv 0$, see Eq. (3.3). In the computational basis, $\hat{\mathcal{H}}_{\text{int}} = -(\hat{\sigma}_A^x + \hat{\sigma}_B^x + \hat{\sigma}_A^x\hat{\sigma}_B^x - \hat{\sigma}_A^y\hat{\sigma}_B^y)$ is of the form

$$\hat{\mathcal{H}}_{\text{int}} = \begin{pmatrix} 0 & h_{00,01} & h_{00,10} & h_{00,11} \\ h_{01,00} & 0 & 0 & h_{01,11} \\ h_{10,00} & 0 & 0 & h_{10,11} \\ h_{11,00} & h_{11,01} & h_{11,10} & 0 \end{pmatrix}. \quad (\text{C.13})$$

By direct inspection, regardless of the detailed definition of the matrix elements, we observe that the diagonal elements of the matrix $\hat{\mathcal{H}}_{\text{int}}\pi_{\hat{u}}$ are identically null, which trivially proves that $E_c^{(g)} = \text{Tr}[\hat{\mathcal{H}}_{\text{int}}\pi_{\hat{u}}] = 0$.

In conclusion, considering the above results, for the g -JQB we simply use $\hat{\mathcal{U}}_g$, since we can neglect $\hat{u}$ in Eq. (C.10) as well as the arbitrary phases of Eq. (2.17), the ergotropy being extracted globally.

C.2.3 Energy spectrum of the two-qubit Hamiltonian in Eq. (3.11)

In the computational basis, the matrix representation of the Hamiltonian in Eq. (3.11) is

$$\hat{\mathcal{H}} = \begin{pmatrix} 2 & -\gamma_0 & -\gamma_0 & -2\gamma_0 \\ -\gamma_0 & 0 & 0 & -\gamma_0 \\ -\gamma_0 & 0 & 0 & -\gamma_0 \\ -2\gamma_0 & -\gamma_0 & -\gamma_0 & -2 \end{pmatrix}, \quad (\text{C.14})$$

whose characteristic polynomial reads

$$p_{\hat{\mathcal{H}}}(\epsilon) = \det(\hat{\mathcal{H}} - \epsilon \hat{I}) = \epsilon[\epsilon^3 - 4(1 + 2\gamma_0^2)\epsilon + 8\gamma_0^3]. \quad (\text{C.15})$$

Therefore, the (unsorted) energy levels are

$$\{\epsilon_k\}_{k=1,\dots,4} = \left\{ 0, \frac{4\sqrt{1+2\gamma_0^2}}{\sqrt{3}} \cos \left[\frac{\phi + 2\pi n}{3} \right] \right\} \quad (\text{C.16})$$

with $n = 0, 1, 2$ and

$$\phi = \arccos \left[-\frac{3\sqrt{3}\gamma_0^3}{2(1+2\gamma_0^2)^{3/2}} \right]. \quad (\text{C.17})$$

The three real roots of the depressed cubic equation, $\epsilon^3 - 4(1 + 2\gamma_0^2)\epsilon + 8\gamma_0^3 = 0$, are obtained via a trigonometric approach [238]. Note that the lowest, ϵ_1 , and the highest, ϵ_4 , energy levels are respectively associated with $n = 1$ and $n = 0$, see Fig. C.2.

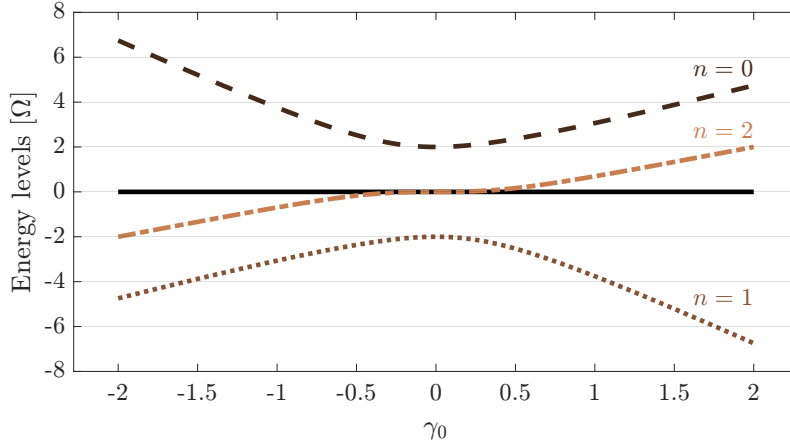


Figure C.2: Spectrum (C.16) of the two-qubit Hamiltonian in Eq. (3.11). Image taken from [22].

Appendix D

Complements to Chapter 4

D.1 Considerations about experimental feasibility

In this Appendix we comment about the fact that the ideal platform to test the functioning of the device discussed in Chapter 4 is represented by a quantum LC circuit (see Section 1.2.3), playing the role of the QB, embedded in an dissipative environment.

The essence of the Caldeira-Leggett model is to replace a linear dissipative element characterized by a frequency dependent admittance $Y(\omega)$ by an infinite set of LC oscillators [169], all wired in parallel, with a properly designed distribution of parameters $\{L_k, C_k\}$ (see the scheme in Fig. D.1). The particular choice of L_k and C_k allows to fine tune the shape of the admittance $Y(\omega)$. This infinite set of oscillators leads the admittance to acquire both an imaginary and a real contribution, ultimately responsible for dissipation. The validity of this approach in the framework of quantum thermodynamic studies based on quantum circuits has been recently discussed in Refs. [185, 186], where indeed the authors have mimicked the behavior of a heat bath in terms a huge number of LC oscillators, eventually terminated with a resistive element and with properly distributed parameters, coupled with the quantum system under investigation (a qubit in their case).

Following the analysis performed in Section 1.2.3, we get Eq. (1.61), that is equivalent to Eq. (2.33). Considering the dissipative part of the circuit, the charge stored in each capacitor is $Q_k(t) = C_k V_k(t)$, while the current going through the inductors is $I_k(t) = L_k^{-1}[\phi(t) - \phi_k(t)]$, with

$$\phi_k(t) = \int_0^t V_k(t') dt'. \quad (\text{D.1})$$

Proceeding in full analogy with what done in Section 1.2.3, one has that the total energy stored in this part of the circuit can be written as [169, 173]

$$U_{\text{diss}}(t) = \sum_k \left\{ \frac{Q_k^2(t)}{2C_k} + \frac{[\phi_k(t) - \phi(t)]^2}{2L_k} \right\}. \quad (\text{D.2})$$

As can be seen, now $\phi(t)$ plays the role of a overall *offset* for the inductive part.

Through the identifications

$$Q_k \leftrightarrow \frac{c_k}{m_k \omega_k^2} \hat{p}_k, \quad \phi_k \leftrightarrow \frac{m_k \omega_k^2}{c_k} \hat{x}_k, \quad (\text{D.3})$$

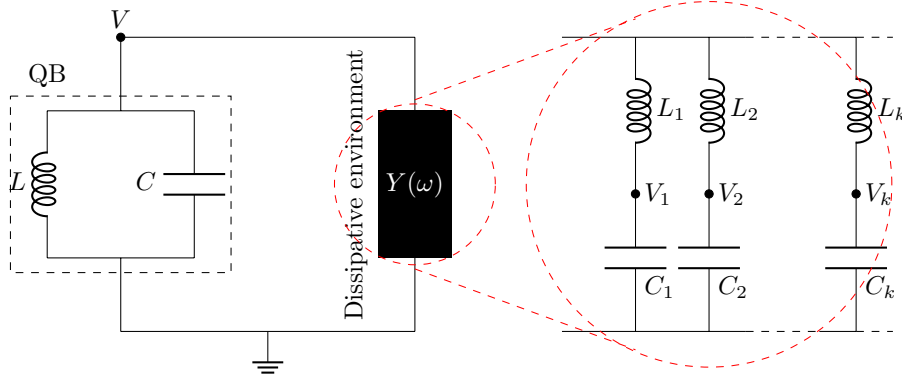


Figure D.1: The quantum LC circuit, playing the role of the QB, is coupled to a dissipative environment (black box). Within the Caldeira-Leggett model the latter, characterized by an admittance $Y(\omega)$, is described in terms of an infinite set of LC oscillators in parallel, with properly distributed parameters L_k and C_k . Here, V and V_k denote the (generally time dependent) voltages associated to the corresponding nodes. Image taken from [36].

and

$$C_k \leftrightarrow \frac{c_k^2}{m_k \omega_k^4}, \quad L_k \leftrightarrow \frac{m_k \omega_k^2}{c_k^2}, \quad (\text{D.4})$$

satisfying $\omega_k = 1/\sqrt{L_k C_k}$, one finally obtains [239]

$$\begin{aligned} \frac{1}{2} \sum_k \left[\frac{\hat{p}_k^2}{m_k} + \frac{c_k^2}{m_k \omega_k^2} \left(\frac{m_k \omega_k^2}{c_k} \hat{x}_k - \hat{x} \right)^2 \right] &= \sum_k \left(\frac{\hat{p}_k^2}{2m_k} + \frac{m_k \omega_k^2}{2} \hat{x}_k^2 - c_k \hat{x}_k \hat{x} + \frac{1}{2} \frac{c_k^2}{m_k \omega_k^2} \hat{x}^2 \right) \\ &= \hat{\mathcal{H}}_R + \hat{\mathcal{H}}_{\text{int}}, \end{aligned} \quad (\text{D.5})$$

as can be seen by comparison with Eqs. (4.2)-(4.5).

On the other hand, for such an environment it is known that, in the time domain, the admittance can be written as [173]

$$Y(t) = \sum_k \frac{1}{L_k} \cos(\omega_k t). \quad (\text{D.6})$$

According to the previous identifications of Eq. (1.59) and Eq. (D.4) this allows, for the times $t \geq 0$ relevant to our dynamics, to identify

$$\frac{Y(t)}{C} \leftrightarrow \gamma(t), \quad (\text{D.7})$$

where the damping kernel $\gamma(t)$ has been defined in Eq. (4.10). In the frequency domain, we also note that the real part of the admittance is related to the spectral density $J(\omega)$ given in Eq. (4.22) by

$$\text{Re}\{Y(\omega)\} = \frac{J(\omega)}{\omega}. \quad (\text{D.8})$$

Owing to the already mentioned identifications, this allows to conclude that in our model

$$\text{Re}\{Y(\omega)\} = C \gamma_0 \frac{\omega_D^2}{\omega^2 + \omega_D^2}. \quad (\text{D.9})$$

Let us now estimate typical parameters for the QB and for the environment.

Concerning the QB, one can assume for example values of $L \approx 50 \mu\text{H}$ for the inductance and $C \approx 5 \text{ pF}$ for the capacity in such a way that the QB can be described as a quantum harmonic oscillator with characteristic frequency $\omega_0/2\pi \approx 10 \text{ MHz}$ (with $\omega_0 = 1/\sqrt{LC}$) [169, 240]. Note that these values are comparable to those used in real state-of-the-art experiments with superconducting LC circuits [241]. Focusing on this frequency regime, which is typically smaller with respect to what usually considered in circuit QED experiments [242], has the practical advantage to allow a control of the device on a time scale in the nanosecond range which is compatible with the discussed features of the figures of merits (the first maximum of η_W occurring at $t_0 \approx 1 \text{ ns}$ assuming for example $\gamma_0 = 300\omega_0$ and $\omega_D = 2\omega_0$ as in Fig. 4.3). The possibility to observe the discussed phenomenology is also assured by its great stability with respect to thermal effect as long as $T \lesssim \Omega$ (see Fig. 4.6). Within the discussed range of parameters this leads to the threshold temperature $T \approx 12 \text{ mK}$ compatible with the cryogenic temperatures typically reached in quantum transport and quantum computing experiments carried out in solid-state devices.

As for the environment, Eq. (D.9) can be identified as the real part of the admittance of a series RL circuit with resistance R_E and impedance L_E given respectively by

$$R_E = \frac{1}{C\gamma_0} \quad ; \quad L_E = \frac{R_E}{\omega_D}. \quad (\text{D.10})$$

For $\omega \ll \omega_D$ the environment behaves ohmically, while for higher frequencies $\omega \gtrsim \omega_D$ the inductive component induces a frequency roll-off.

From the estimates given above one can obtain typical values $R_E \approx 10 \Omega$ and $L_E \approx 500 \text{ nH}$. To conclude, we note that quantum couplers can be used to realize a fast control of the coupling between the QB and the charger [130–132].

D.2 The response function $\chi(t)$ in the strong underdamped regime

In this Appendix we give some details on the behavior of the response function $\chi(t)$.

The cubic equation in Eq. (4.28)

$$\lambda^3 - \lambda^2\omega_D + \lambda(\omega_0^2 + \gamma_0\omega_D) - \omega_D\omega_0^2 = 0 \quad (\text{D.11})$$

yields the general Vieta's relations

$$\lambda_1 + \lambda_2 + \lambda_3 = \omega_D, \quad (\text{D.12})$$

$$\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3 = \omega_0^2 + \gamma_0\omega_D, \quad (\text{D.13})$$

$$\lambda_1\lambda_2\lambda_3 = \omega_D\omega_0^2. \quad (\text{D.14})$$

We remind that, for finite damping, all roots have positive real parts. In addition, in the underdamped regime two roots are complex and one is real, so they can be written as

$$\lambda_{1,2} = \Gamma \pm i\nu, \quad \lambda_3 \in \mathbb{R}, \quad (\text{D.15})$$

where $\Gamma, \nu \in \mathbb{R}$. Using Eqs. (D.12) and (D.14) we have

$$\Gamma = \frac{\omega_D - \lambda_3}{2}, \quad \Gamma^2 + \nu^2 = \frac{\omega_D \omega_0^2}{\lambda_3}. \quad (\text{D.16})$$

According to this, the χ_j defined in Eq. (4.29) are

$$\chi_1 = \frac{i}{2\nu} \left[\frac{2\nu + i(\lambda_3 + \omega_D)}{2\nu + i(3\lambda_3 - \omega_D)} \right], \quad \chi_2 = \chi_1^* \quad (\text{D.17})$$

$$\chi_3 = 4 \frac{\omega_D - \lambda_3}{(\omega_D - 3\lambda_3)^2 + 4\nu^2}. \quad (\text{D.18})$$

We now derive analytic expressions at strong coupling with $\gamma_0 \gg \omega_D, \omega_0$, that is $\Omega = \sqrt{\gamma_0 \omega_D} \gg \omega_0, \omega_D$. Here, to leading order in Ω , the real the solution of Eq. (D.11) is

$$\lambda_3 \approx \frac{\omega_0^2 \omega_D}{\Omega^2}. \quad (\text{D.19})$$

Inserting this results in Eqs. (D.16) one has

$$\Gamma \approx \frac{\omega_D}{2}, \quad \nu \approx \Omega. \quad (\text{D.20})$$

Concerning χ_j we find

$$\chi_1 \approx \frac{i}{2\Omega} \left[1 + i \frac{\omega_D}{\Omega} \right], \quad \chi_2 = \chi_1^*, \quad \chi_3 \approx \frac{\omega_D}{\Omega^2}. \quad (\text{D.21})$$

This leads to the following expression for the response function $\chi(t) = \sum_j \chi_j e^{-\lambda_j t}$

$$\chi(t) \approx \frac{e^{-\frac{\omega_D}{2}t}}{\Omega} \left[\sin(\Omega t) - \frac{\omega_D}{\Omega} \cos(\Omega t) \right] + \frac{\omega_D}{\Omega^2} e^{-\frac{\omega_0^2 \omega_D}{\Omega^2} t}, \quad (\text{D.22})$$

whose leading order expansion is

$$\chi(t) \approx \frac{e^{-\frac{\omega_D}{2}t}}{\Omega} \sin(\Omega t) \quad (\text{D.23})$$

as quoted in Eq. (4.31).

D.3 Explicit expression for QB variances

In this Appendix we give details on how to get the general expressions of the variances $\langle x^2(t) \rangle$ and $\langle \dot{x}^2(t) \rangle$ quoted in the main text – see Eqs. (4.39) and (4.40).

We start by recalling that the solution of the Langevin equation (4.9) can be decomposed as $\hat{x}(t) = \hat{x}_h(t) + \hat{x}_{th}(t)$: this will be the building block for evaluating the above quantities. The homogeneous part is given by

$$\hat{x}_h(t) = \hat{\dot{x}}(0)\chi(t) + \hat{x}(0)\dot{\chi}(t), \quad (\text{D.24})$$

while the thermal one is

$$\hat{x}_{th}(t) = \int_0^t \frac{dt'}{m} \chi(t-t') \hat{\xi}(t'), \quad (\text{D.25})$$

which, due to the initial condition $\chi(0) = 0$ implies also

$$\hat{x}_{\text{th}}(t) = \int_0^t \frac{dt'}{m} \dot{\chi}(t-t') \hat{\xi}(t'). \quad (\text{D.26})$$

Here, the dot represents the derivative with respect to the first argument.

On a very general ground, given initial decoupled conditions and

$$\langle \hat{\xi}(t) \rangle = \langle \hat{x}(t) \rangle = 0, \quad \langle \dot{\hat{x}}(t) \rangle = 0, \quad (\text{D.27})$$

the homogeneous and thermal terms factorize as

$$\begin{aligned} \langle \hat{x}^2(t) \rangle &= \langle \hat{x}_{\text{h}}^2(t) \rangle + \langle \hat{x}_{\text{th}}^2(t) \rangle, \\ \langle \dot{\hat{x}}^2(t) \rangle &= \langle \dot{\hat{x}}_{\text{h}}^2(t) \rangle + \langle \dot{\hat{x}}_{\text{th}}^2(t) \rangle. \end{aligned} \quad (\text{D.28})$$

These matrix elements completely define the contributions to the covariance matrix $\sigma_{\text{B}}(t) = \sigma_{\text{B,h}}(t) + \sigma_{\text{B,th}}(t)$ given by

$$\sigma_{\text{B,h/th}}(t) = m \begin{pmatrix} \omega_0 \langle \hat{x}_{\text{h/th}}^2(t) \rangle & \frac{1}{2} \frac{d}{dt} \langle \hat{x}_{\text{h/th}}^2(t) \rangle \\ \frac{1}{2} \frac{d}{dt} \langle \hat{x}_{\text{h/th}}^2(t) \rangle & \frac{1}{\omega_0} \langle \dot{\hat{x}}_{\text{h/th}}^2(t) \rangle \end{pmatrix}. \quad (\text{D.29})$$

We now observe that the homogeneous part is independent of the temperature and can be easily written in term of the response function $\chi(t)$. Taking into account the initial conditions and using Eq. (D.24) one straightforwardly arrives to the expressions

$$\begin{pmatrix} \langle \hat{x}_{\text{h}}^2(t) \rangle \\ \langle \dot{\hat{x}}_{\text{h}}^2(t) \rangle \end{pmatrix} = \frac{\omega_0}{2m} \begin{pmatrix} \chi^2(t) \\ \dot{\chi}^2(t) \end{pmatrix} + \frac{1}{2m\omega_0} \begin{pmatrix} \dot{\chi}^2(t) \\ \ddot{\chi}^2(t) \end{pmatrix}. \quad (\text{D.30})$$

As expected, $\sigma_{\text{B,h}}(t \rightarrow \infty) = 0$.

Concerning the thermal contributions we need a more careful manipulation of Eqs. (D.25) and (D.26). In the following we describe how to explicitly write $\langle \hat{x}_{\text{th}}^2(t) \rangle$.

Using Eq. (D.25) we have

$$\langle \hat{x}_{\text{th}}^2(t) \rangle = \frac{1}{m^2} \int_0^t dt_1 \int_0^t dt_2 \chi(t-t_1) \chi(t-t_2) \langle \hat{\xi}(t_1) \hat{\xi}(t_2) \rangle \quad (\text{D.31})$$

Since the integrand is symmetric under exchange of t_2 with t_1 , only the symmetric part of the correlation function $\langle \hat{\xi}(t_1) \hat{\xi}(t_2) \rangle$ contributes. We call it [243, 244]

$$\mathcal{L}_s(t_1 - t_2) = \int_0^\infty \frac{d\omega}{\pi} J(\omega) \coth\left(\frac{\beta\omega}{2}\right) \cos[\omega(t_1 - t_2)], \quad (\text{D.32})$$

see Eq. (4.38), with Fourier transform

$$\mathcal{L}_s(\omega) = J(\omega) \coth\left(\frac{\beta\omega}{2}\right). \quad (\text{D.33})$$

Inserting now the general expression of $\chi(t)$, given in Eq. (4.27), and integrating over time one finally obtains

$$\begin{aligned} \langle \hat{x}_{\text{th}}^2(t) \rangle &= \sum_{j,j'=1}^3 \chi_j \chi_{j'} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi m^2} \frac{\mathcal{L}_s(\omega)}{(\lambda_j - i\omega)(\lambda_{j'} + i\omega)} \\ &\quad \left[1 - e^{-(\lambda_j - i\omega)t} - e^{-(\lambda_{j'} + i\omega)t} + e^{-(\lambda_j + \lambda_{j'})t} \right]. \end{aligned} \quad (\text{D.34})$$

The last term to be evaluated is $\langle \hat{x}_{\text{th}}^2(t) \rangle$. This follows straightforwardly by inserting the expression in Eq. (D.26) which gives

$$\langle \hat{x}_{\text{th}}^2(t) \rangle = \frac{1}{m^2} \int_0^t dt_1 \int_0^t dt_2 \dot{\chi}(t-t_1) \dot{\chi}(t-t_2) \langle \hat{\xi}(t_1) \hat{\xi}(t_2) \rangle. \quad (\text{D.35})$$

Following similar steps as done for $\langle \hat{x}_{\text{th}}^2(t) \rangle$ a form similar to Eq. (D.34) is found, except for the substitutions $\chi_j \cdot \chi_{j'} \rightarrow \lambda_j \chi_j \cdot \lambda_{j'} \chi_{j'}$, see also Eq. (4.40)

$$\begin{aligned} \langle \hat{x}_{\text{th}}^2(t) \rangle &= \sum_{j,j'=1}^3 \lambda_j \chi_j \lambda_{j'} \chi_{j'} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi m^2} \frac{\mathcal{L}_s(\omega)}{(\lambda_j - i\omega)(\lambda_{j'} + i\omega)} \\ &\quad \left[1 - e^{-(\lambda_j - i\omega)t} - e^{-(\lambda_{j'} + i\omega)t} + e^{-(\lambda_j + \lambda_{j'})t} \right]. \end{aligned} \quad (\text{D.36})$$

We close this Section by commenting on the long time limit. For $t \rightarrow +\infty$ only the first term in the squared brackets of $\langle \hat{x}_{\text{th}}^2(t) \rangle$ and $\langle \hat{x}_{\text{th}}^2(t) \rangle$ survives (see Eqs. (D.34) and (D.36)) since $\text{Re}\{\lambda_j\} > 0$. Then, after some manipulations, we arrive to the form

$$\begin{aligned} \langle \hat{x}_{\text{th}}^2(+\infty) \rangle &= \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi m} \coth\left(\frac{\beta\omega}{2}\right) \text{Im} [\tilde{\chi}(\lambda = -i\omega)] , \\ \langle \hat{x}_{\text{th}}^2(+\infty) \rangle &= \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi m} \omega^2 \coth\left(\frac{\beta\omega}{2}\right) \text{Im} [\tilde{\chi}(\lambda = -i\omega)] . \end{aligned} \quad (\text{D.37})$$

In addition, we can easily see from Eq. (D.34) that

$$\lim_{t \rightarrow \infty} \frac{d}{dt} \hat{x}_{\text{th}}^2(t) = 0. \quad (\text{D.38})$$

This confirms the expected fluctuation-dissipation theorem [64].

D.4 State of the QB at maximum efficiency and possible work extraction

In this Appendix we characterize in more details the state of the QB by means of its Wigner function [245, 246]

$$\mathcal{W}(x, p, t) = \frac{1}{2\pi \sqrt{\text{Det}[\sigma_{\text{B}}(t)]}} e^{-\frac{1}{2} \mathbf{r}^t \sigma_{\text{B}}^{-1}(t) \mathbf{r}}, \quad (\text{D.39})$$

where $\mathbf{r}^t = (x, p)$ is the (transposed) vector of the variables x and p in the QB quantum phase space. Right before the QB is coupled to the charger it sits in its ground state, shown in panel D.2(a). In correspondence of the first maxima of the efficiencies (η_B and η_W), the state of the QB is instead very close to an extremely squeezed state along the momentum direction, as clearly shown in panel (b) of the above figure - please notice the change in scales between the two panels.

From this observation, one can infer that an unitary operation able to almost completely extract the energy from the QB is an "anti-squeezing" operator, namely

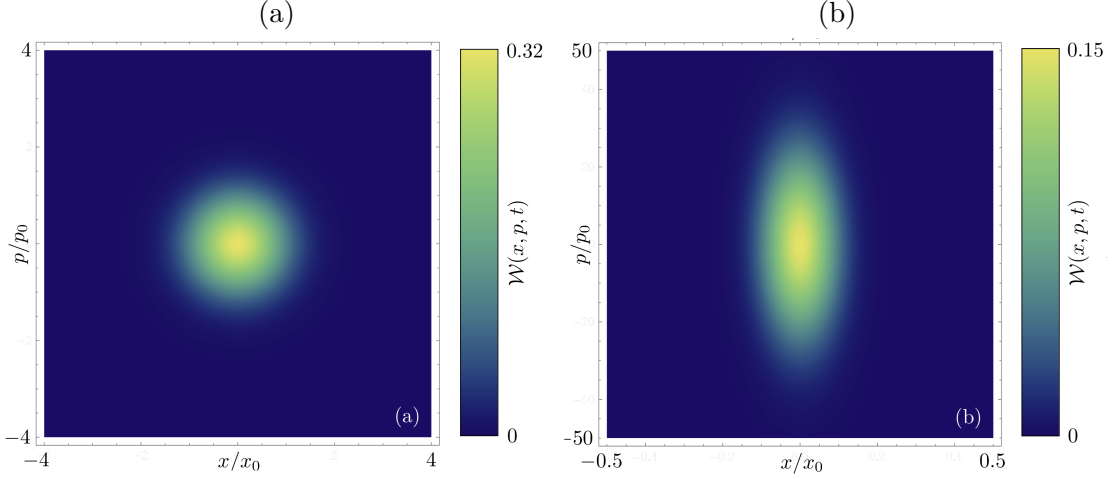


Figure D.2: Plot of $\mathcal{W}(x, p, t)$ (units $\hbar^{-1} = 1$) as a function of x (units $x_0 = \sqrt{\frac{\hbar}{2m\omega_0}}$) and p (units $p_0 = \sqrt{\frac{\hbar m\omega_0}{2}}$). Here, darker (lighter) colors denote smaller (larger) values. Panel (a) shows the Wigner function of the QB in its ground state right before coupling to the charger ($t = 0$). Panel (b) represents it in correspondence of the first maxima of the efficiencies η_B and η_W . It is worth to note that the axis scales of the two figures differ by a factor of about 10. The considered parameters are $\omega_D = 2\omega_0$ (corresponding to $\Omega \approx 24.5\omega_0$) and $\gamma_0 = 300\omega_0$, $T = 0.1\omega_0$. Image taken from [36].

the hermitian conjugate of the conventional squeezing operator $\hat{S}(\xi) = e^{\frac{1}{2}[\xi^*(\hat{a})^2 - \xi(\hat{a}^\dagger)^2]}$, where $\hat{a}$ and $\hat{a}^\dagger$ are the ladder operators associated to $\hat{x}$ and $\hat{p}$ and where ξ is a squeezing parameter which, in the present case, depends on the action of the reservoir during the charging phase. This operation is able to bring the QB very close to the initial ground state. This kind of operation has been discussed in other platforms, such as quantum optics, under the name of deamplification [247] and could be implemented also in solid-state devices exploiting for example exotic two-photon interaction [222].

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