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QUANTUM BATTERIES BASED ON METASTABLE MOLECULES

Yordan KATSAROV

"Georgi Benkovski", Bulgarian Air Force Academy, Dolna Mitropolia, Bulgaria
yordankatsarov@gmail.com

Abstract: *Quantum batteries (QB) are still experimental, but their potential to revolutionize energy storage is immense. This work provides a thorough physical explanation and investigation into the possible practical realization of energy storage. The core idea is to use metastable molecules and the rules of forbidden transitions to store energy in the excited state for an extended period. Metastable states are unique because they allow systems to remain in non-equilibrium conditions for extended periods before transitioning to stable states. Metastability also offers protection against dissipation and decoherence; however, its application in QB remains largely unexplored. The potential of the "Pentacene 5b and 5c" molecules has been explored as a practical realization of QB.*

Keywords: metastable, decoherence, entanglement, excited state

1. Introduction

QB is a device that utilizes quantum-mechanical effects to store and release energy, unlike conventional batteries that depend on chemical reactions. QB captures energy by exciting atoms or molecules and storing it as photons or in excited states instead of through chemical bonds. This approach enables QB to harness exotic quantum phenomena such as superposition and entanglement, where particles can exist in multiple states or interact to achieve performance capabilities that surpass classical limits. Physicists Alicki R. and Fannes M. proposed the concept in 2013 [1]. The interaction of a particle with the environment creates entanglement. This correlation is, in practical sense information and can be used as energy [2]. Dicke first model was in 2018 [3-6] and initially appeared to demonstrate a quantum advantage in charging power. However, subsequent research revealed that modifications to its Hamiltonian (H) were necessary, ultimately indicating that the model does not provide any quantum advantage. The semi-classical limit and chaos have appeared [7-13]. This model uses dipole coupling and interaction with a single-mode cavity. The coupling permits the atoms to exchange energy with the cavity field, leading to phenomena such as a superradiant phase transition. However, achieving this interaction experimentally can be challenging due to weak coupling and theoretical limitations, often addressed using external pumps and effective models [14, 15]. This first model is fundamentally important for elucidating the collective behaviour of atoms interacting with a single electromagnetic mode [16]. The study by Rossini et al. in 2020 [17] introduced a model for a many-body QB, demonstrating a clear quantum advantage. This advantage is associated with super-extensive scaling - a phenomenon where the charging power increases faster than the number of battery cells [18]. Rossini et al. specifically

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investigated the Sachdev-Ye-Kitaev (SYK) model [19, 20], which utilizes strong quantum correlations to improve charging efficiency. Different systems, like quantum dots, topological superconductors, graphene flakes, and optical lattices, were suggested for QB models. [21-23]. Some variations of the model are suitable for digital quantum simulation [24], with pioneering experiments conducted in nuclear magnetic resonance [25]. Charging occurs through the complex c-SYK Hamiltonian, indicating that non-local Jordan-Wigner fermion model are fundamental [26]. A "good" battery should not only charge rapidly but also be able to deliver this energy effectively [27, 28]. It is important to highlight that the concept of energy extraction has been investigated within the framework of waveguide quantum electrodynamics, as explored in [29, 30], and in the context of random quantum systems, as discussed in [31]. Although achieving efficient charging and energy extraction remains a priority, it should be noted that speed may compromise precision [32-35].

This study employs a novel method involving metastable molecules by keeping energy for an extended period in population inversion excited state, drawing inspiration from the research conducted by Wang et al. [36].

2. Theoretical Background

2.1. Energy at the Quantum Level

Extracting work and generating work are different concepts in thermodynamics and quantum mechanics. Even though quantum effects exist, the laws of thermodynamics still apply, (see Fig. 1).

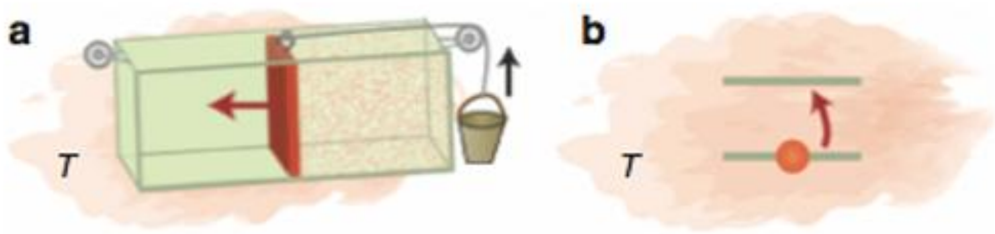

Figure 1: **a***: Classical thermodynamic work is a potential energy.* **b***: In quantum thermodynamics, one bit of work is the transition from one energetic level to another. (Figure taken from Nature Comm. 4 2059 (2013).).*

2.2. The First Law of Thermodynamics

$$\langle Q\rangle+\langle W\rangle = \int_0^{\tau} \frac{d}{dt}\,\mathrm{tr}\left[\rho^{(t)}H^{(t)}\right]\mathrm{d}t =$$

$$= \mathrm{tr}\left[\rho^{(\tau)}H^{(\tau)}\right] - \mathrm{tr}\left[\rho^{(0)}H^{(0)}\right] = \Delta U \qquad (1)$$

where: ρ - quantum state; H – Hamiltonian, vary in time $t\epsilon(0,\tau)$; U(ρ) = tr[ρH] - *expectation value*; ΔU – *average energy change*; Q - heat; W- work; tr - trace.

2.3. The Second Law of Thermodynamics

A fundamental law of physics it limits the work extraction of heat engines and establishes the notion of irreversibility in physics.

$$\int \frac{\langle \delta Q\rangle}{T} \leq \Delta S_{th} \qquad (2)$$

where: $\langle \delta Q\rangle$ - heat absorbed along the process; T - temperature; S_{th} - thermodynamic entropy.

2.4. Free Energy

Clausius' inequality defines an upper limit on the heat absorbed by a system, and its applicability is commonly presumed to extend into the quantum domain.

$$F(\rho) := \mathrm{U}(\rho) - TS_{th}(\rho) \qquad (3)$$

where $F(\rho)$ is the *free energy* of a system.

2.5. Network Batteries and Spin-Chain

The model, first proposed by Le et al. [38], of a many-body QB. Spin chain is a one-dimensional array consist of two-level systems (TLSs). TLSs can be charged and discharged through quantum operations, such as unitary transformations (see Fig. 2).

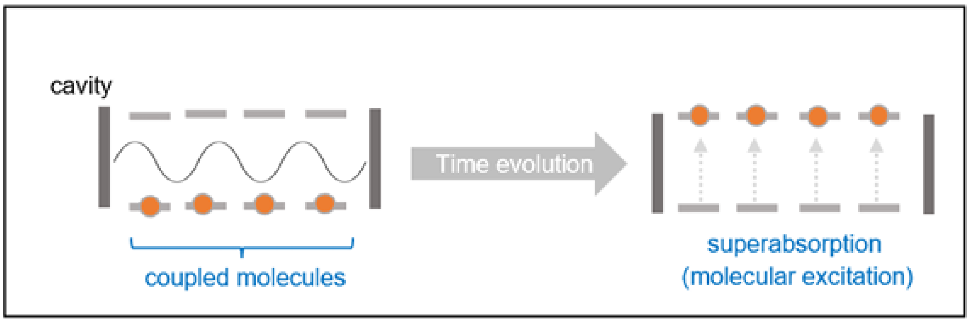

Figure 2: A scheme of charging a quantum battery through superabsorption, comprising multiple work qubits. The superposition states are induced by enhancing the couplings between the work qubits by stimulation. (Figure taken from Journal of the Physical Society of Japan, Volume 91, Number 12, Quantum Battery Based on Superabsorption [37].).

2.6. Hamiltonians

The total H generates the dynamics of an open quantum battery (OQB) is:

$$H = H_B + H_C + H_E + H_{int} \quad (4)$$

where H_B is battery; H_C is charger; H_E is environment; H_{int} is interaction part.

2.6.1. Dicke Hamiltonian

It is the collective interaction between an ensemble of N two-level system (TLS) atoms and a single mode of the cavity field:

$$H_{Dicke} = \omega_c \hat{a}^\dagger \hat{a} + \omega_0 \sum_{i=1}^{N} \hat{\sigma}_i^z + +g \sum_{i=1}^{N} \hat{\sigma}_i^x (\hat{a}^\dagger + \hat{a}) \quad (5)$$

were: $\hat{a}\hat{a}^\dagger$ annihilate (create) photons; ω_c - frequency; ω_0 - resonant frequency; $\hat{\sigma}_i^\alpha$ - Pauli operators; g -cavity coupling parameter. Cavities - generally constructed using two mirrors that reflect light repeatedly, generating electromagnetic standing wave.

2.6.2. SYK Model

Rossini et al. [17] take SYK for its model. Where charging went via a direct charging protocol. The internal battery $H_0^{(N)}$ is a sum of local terms, given by:

$$H_B^{(0)} = \omega_0 \sum_{i=0}^{N} \hat{\sigma}_i^y \quad (6)$$

and (c-SYK) charging Hamiltonian ,

$$H_B^{(1)} = \sum_{i,j,k,l=0}^{N} J_{i,j,k,l} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k \hat{c}_l \quad (7)$$

where $\hat{c}_j^\dagger$ ($\hat{c}_j$) is a spinless fermionic creation (annihilation) operator; $J_{i,j,k,l}$ are zero-mean Gaussian-distributed complex random variables.

2.6.3. Local and Nonlocal Interactions

Rosa et al. [39] discuss the many-body QB. They consider the standard, local N-spin battery, with H_i = h$\hat{\sigma}_i^z$ (h-energy scale of each subsystem). The authors present a two-model for the interaction $H_1^{(N)}$:

$$H_{MBL}^{(N)} = \sum_{i=1}^{N} (J_{i,j,k,l}\, \hat{\sigma}_j^x \hat{\sigma}_{j+1}^x + J_2 \hat{\sigma}_j^x \hat{\sigma}_{j+2}^x) \quad (8)$$

$$H_{SYK}^{(N)} = \sum_{i<j<k<l}^{N} J_{i,j,k,l}\, \hat{\gamma}_i \hat{\gamma}_j \hat{\gamma}_k \hat{\gamma}_l \quad (9)$$

here: J_j and J_2 are Ising couplings; $\hat{\gamma}_i$ - Majorana fermion operator.

Bought internal $H_0^{(N)}$ with many-body *localized* $H_{MBL}^{(N)}$ serves as a model for many-body quantum systems. The $H_{SYK}^{(N)}$ is characterized by *non-local* all-to-all random interactions that promote the formation of highly entangled states. Since SYK models can provide both powerful and precise charging [17, 39], the next step should focus on experimentally feasible SYK charging architectures.

2.7. Metastable States and Forbidden Transitions

In quantum physics, certain excited states of atoms or molecules are extremely long-lived because direct transitions to lower states are "*forbidden*" by selection rules. In a typical atom, when an electron is excited to a higher orbital, it will spontaneously decay back to the ground state by emitting a photon, usually within nanoseconds.

However, if the decay process requires a change in the electron's state that violates fundamental selection rules (such as conservation of angular momentum or spin) the transition cannot proceed via the usual fast route (electric dipole emission). Such an excited state is called a *metastable state* (see Fig. 3) – it will eventually decay via higher-order processes (magnetic dipole, electric quadrupole, two-photon emission, etc.), but on timescales that can be orders of magnitude longer than normal. In other words, the state is an energy "trap", holding the excitation energy for an extended period.

This principle is at the heart of the QB model – one wants to excite atoms/molecules and have them remain excited (charged) for as long as possible. Campaioli et al. [40] first suggested harnessing the protective nature of metastability to reduce energy loss in OQB.

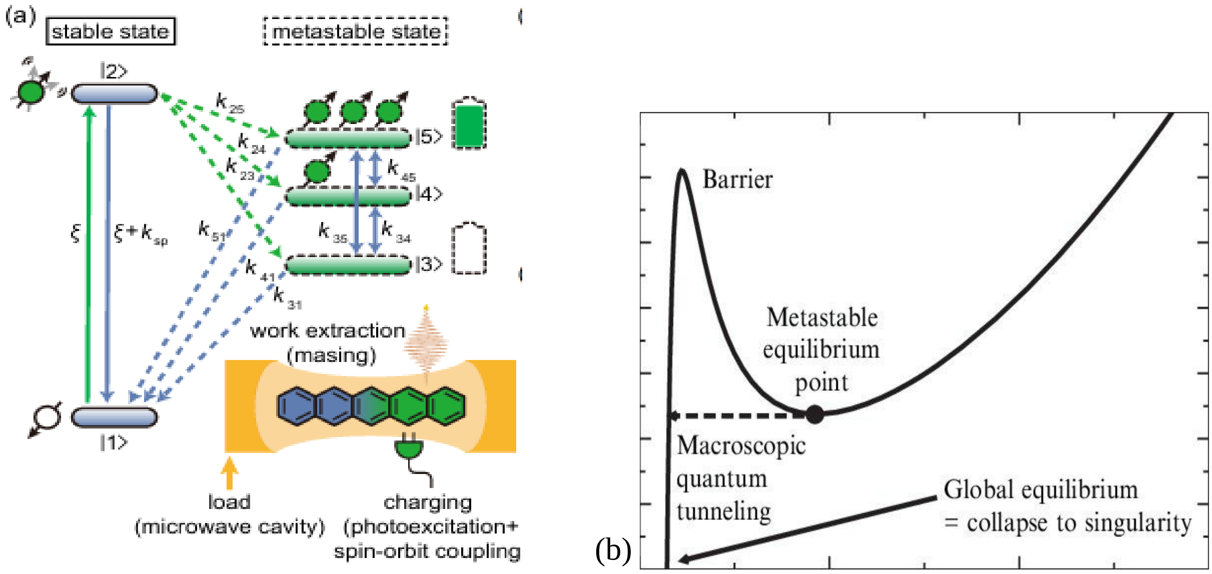

Figure 3: (a).Mechanism of the metastability-induced solid-state quantum battery. General mechanism illustrating the quantum battery based on the metastable triplet states (dashed green boxes) formed via the intersystem crossing from the photo-excited singlet states (solid blue boxes). (b). Metastability with macroscopic quantum tunneling. (Figures taken from: (a) Quantum Physics [36]; (b) Emergent Nonlinear Phenomena in Bose-Einstein Condensates. Theory and Experiment. Book ©2008.)

3. Results and Discussion

3.1. Theoretical.

The main idea of this work is a new model, referred to as QB, which is inherently inclined to metastable molecular states. These molecules are excited by light in the high-frequency spectrum and maintained in a prolonged excited state through the constant magnetic field. It utilizes population inversion, supported by the rules of forbidden transitions, to effectively retain energy. At last, almost every chemical element has one metastable excited state. The presence of metastable levels is evident in atomic spectra due to selection rules that forbid specific transitions to lower energy states. These states were effectively accessed through pumping methods, such as electrical discharge or optical excitation with lasers. One can further use external fields to manage these metastable states. A static magnetic field, for instance, can lift degeneracies and define a quantization axis (the Zeeman Effect), which helps in two ways: (1) it can allow us to address specific transitions with lasers (by separating levels that were otherwise too close or forbidden), and (2) it can prevent unwanted transitions by disallowing certain polarization couplings. In our context, we might do the reverse – use the magnetic field to maintain the forbiddingness of the transition during storage, but possibly remove or alter the field when we want to actively induce emission (discharge). The key point is that metastable states often involve specific spin or angular momentum configurations, and a magnetic field can stabilize those configurations. Thus, a combination of selection rules and magnetic fields provides a toolbox for creating a long-lived "charged" quantum state, well isolated from environmental disturbances and spontaneous emission. This forms the theoretical foundation for a quantum battery composed of light-pumped metastable molecules.

3.2. Experimental Realization.

Benzo-cyclohepta-fluorene (**5a**), a new π-conjugated polycyclic hydrocarbon, was designed, and its stable derivatives **5b** and **5c** were synthesized (see Fig. 4). 5a is an *isomer of pentacene*, meaning it shares the same molecular formula but differs in the arrangement of atoms. Unlike pentacene, which consists solely of six-membered rings, 5a incorporates five- and seven-membered rings, giving it distinct electronic and resonance properties. The molecule contains 22 π electrons, contributing to its conjugated system and enabling resonance forms.

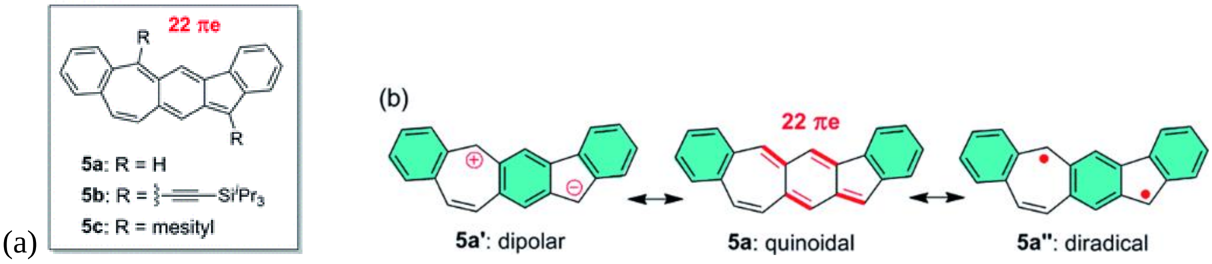

Figure 4: (a) Pentacen chemical structures and their analogues, (b) The typical resonance forms 5a. (Figure taken from journal © The Royal Society of Chemistry 2016.) [41]

Stable derivatives of 5a, named 5b and 5c, were synthesized to enhance their stability. It has also explored their potential as organic semiconductors, with 5b demonstrating π-type semiconducting behavior in thin-film transistors. My proposal is for a pentacene-doped crystal quantum battery that can power a light device. That QB should be at room temperature and with a multi-layer organic structure. In these setups, a population of 5b and 5c molecules is optically pumped. Derivatives 5b and 5c well-known room-temperature triplet state, act as the storage medium. The setup resembles a laser apparatus: a laser excites the object (often a pulsed laser, since a short, intense pulse can simultaneously excite many molecules). The setup includes: a crystal host (to hold a high density of metastable centers), a pumping laser (visible light) typically pulsed to achieve high population inversion, a static magnetic field, a specific crystal orientation (to get the right sublevel structure), and a cavity to extract the emission. The 5b and 5c work as an energy store that can be discharged on demand into the cavity mode. Impressively, these pentacene-based systems operate at room temperature and ambient conditions, unlike many quantum experiments that require ultracold or ultra-high vacuum environments. This underscores the practicality of the approach: by using molecular systems with intrinsic metastability, one can avoid complex cooling or trapping. (In comparison, atomic metastable states often require vacuum chambers and laser cooling/trapping.)

3.3. Discussion.

By pumping molecules with visible light into long-lived excited states and using magnetic fields to enforce forbidden transition rules, one can create miniature energy storage units that defy some limitations of classical batteries. The theoretical principles, through forbidden transitions that yield long-time metastability, to collective quantum effects that speed up charging and discharging, have been validated in multiple experiments on small scales. Molecules like pentacene 5b and 5c have demonstrated that it is possible to charge a quantum battery with a flash of light and, after that, extract the energy as coherent radiation. Novel setups like multi-layer microcavities show that such energy can even be drawn as electrical power, all while exhibiting quantum enhancements in performance. However, translating these advantages to everyday use will require overcoming several challenges. Scalability is a major hurdle: we need to go from prototypes with perhaps $\mathbf{10^{15}}$ molecules storing Pico Joules (J), to macroscopic packs storing J or kJ. That means combining an enormous number of quantum cells while preserving their special properties. Maintaining coherence or at least preventing decoherence from spoiling the stored energy is non-trivial in a large system (environmental interactions tend to increase with system size). Additionally, safety and practicality must be considered – a device that uses lasers and magnetic fields internally must be made as safe and easy to use as a regular battery.

4. Conclusions

In conclusion, the new model of a quantum battery using light-pumped metastable molecules is a shining example of how abstract quantum principles can be harnessed for practical ends. It leverages the fact that nature permits, in very specific circumstances, energy to be stored in a “paused” state – an excited molecule that wants to emit a photon but can’t, due to quantum rules. By assembling many such molecules and coordinating them, we gain a battery that can be charged rapidly (with a flash of light) and that holds its charge until we decide to release it. The journey from laboratory demonstrations to everyday technology is ongoing, but the progress so far is promising. Should these efforts succeed, QB might complement or even compete with chemical batteries, leading to electronics that charge in an eye-blink and energy systems with unprecedented performance. The marriage of laser optics and battery technology under the guidance of quantum physics could truly be transformative, allowing us to “store sunshine in an atom”.

Further work. Practical demonstrations of QB are emerging on multiple fronts. The most advanced prototypes (like the organic molecule micro-cavity battery) show that the whole cycle – fast photon charging, stable energy hold, and controlled discharge – is achievable in a laboratory device. Other experimental efforts in quantum optics are validating the underlying mechanisms, such as entanglement-enhanced charging and metastable storage, on a smaller scale. All evidence so far suggests that the basic concept is sound. The remaining work is to scale up these systems, improve their efficiency, and integrate them into real-world technology.

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