Quantum Molecular Robots

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Living organisms exploit complex molecular machines to execute crucial functions in chaotic environments. Inspired by nature’s molecular setups we explore the idea of a quantum mechanical device whose purpose is self-protecting quantum information against a noisy environment.

INTRODUCTION

Molecules that execute tasks in crowded noisy environments are pervasive in biology. Molecular machines, as they are often called, are complex structures with thousands of atoms self-orchestrated to perform specific functions that draw energy and information from their surroundings to sustain motional and chemical nonequilibrium states essential to life. It is often discussed whether quantum mechanical effects play a role in these phenomena, and it has many times been suggested that coherence and entanglement can improve the efficiency of biomolecular processes. We propose an exploration of the dual question: what lessons can we draw from biology that would improve control over quantum mechanical matter?

Nanotechnology has been largely inspired by nature’s machines. Artificial molecular pumps, motors, and quantum tunneling ratchets and microscopic versions of Maxwell’s demon have been synthesized and studied. Molecular data storage and processing using DNA are also possible, and gene editing technology is now standard. In parallel to developments in nanotechnology, the study of ultracold quantum chemistry has enabled the observation of molecular assembly from single atoms as well as chemical reactions at the single molecule level. Quantum interference of large organic molecules has been demonstrated and it has been argued that the technology for preparing large biological systems in quantum superposition states is within reach.

It is expected that eventually, ultracold quantum chemistry and nanotechnology will merge, perhaps fueled by the upcoming advances in quantum simulation and computation. One could then imagine the experimental realization of quantum molecular machines, which we will refer to as quantum robots, or qubots for short. Inspired by biological molecular machines such as kinesin, RNA Polymerase, and self-replicating ribosomes, qubots draw energy and information from their surroundings with the purpose of maintaining and processing quantum mechanical non-equilibrium states against the detrimental actions of decoherence and thermalization. Similar to naturally occurring machines, such structures have the potential of being significantly complicated, yet nothing prevents them from having molecular dimensions. A qubot can thus be thought of as an active self-error correcting molecule functioning as a quantum memory or processor.

Engineering the environment and exploiting the dynamics of open systems to protect quantum states and achieve fault tolerance is an interesting idea with proposals in quantum information and optics. Moreover, it is known that noise and decoherence are not always detrimental for entangled states, and that autonomous quantum thermal engines can prepare entanglement in the steady state. Topological error correcting codes are also an example of naturally fault tolerant systems. Qubots differ from the idea of an engineered environment and topological codes as they actively draw energy and resources from the external world to protect their quantum data against a pre-existing non-engineered environment. An interesting parallel can be drawn with a quantum error correcting code, where syndrome measurements are made and correction operators are subsequently applied by an external agent. For a qubot, the error detection and correction are intrinsic parts of itself in a similar manner DNA Polymerase performs proofreading and error correction on a strand of DNA.

In this work we explore possibilities around the concept of quantum molecular machines. The main idea is to provide a simple toy example that captures the essence of a qubot. In the following section we construct such an example. Next we give an effective master equation description of the model. A discussion on possible implementations and future perspectives follows.

EXAMPLE OF A QUBOT

We give an example of a quantum robot that stabilizes one e-bit of quantum information in the form of a singlet state against a dephasing environment. The construction can be seen as an algorithm running on an open quantum computer and we will assume the ability to execute two-qubit operations among subsystems.

A ludic drawing of the qubot and its different configurations is shown in Figure 1(a). Consider a pair of particles A, B. These particles will constitute the “nucleus” of the qubot and provide the protected spin degrees of freedom. The particles have spin 1/2, and interact with each other via an interatomic potential of the form

\[ V(R) = V_0(R) + \vec{S}_A \cdot \vec{S}_B \cdot V_1(R) \] (1)
where \( R \) is the inter-particle distance and \( \vec{S}_A, \vec{S}_B \) the particles’ spin operators. The exact form of \( V_0(R) \) and \( V_1(R) \) is not important as long as the potential \( V(R) \) assumes a shape like the sketch shown in Figure 1(b) for the singlet \(|s\rangle\) and triplet \(|t\rangle\) states, defined as

\[
|s\rangle = \frac{\left| \uparrow \right>_A \left| \downarrow \right>_B - \left| \downarrow \right>_A \left| \uparrow \right>_B}{\sqrt{2}} \quad (2)
\]

\[
|t\rangle = \frac{\left| \uparrow \right>_A \left| \downarrow \right>_B + \left| \downarrow \right>_A \left| \uparrow \right>_B}{\sqrt{2}} \quad (3)
\]

Inspired by atomic physics we may say that \( V_0(R) \propto R^{-3} \) and \( V_1(R) \propto R^{-6} \), and particles \( AB \) form a molecular term \( ^1\Sigma^+ \) for the singlet and \( ^3\Sigma^+ \) for the triplet states [14].

Around the particles \( AB \) there is a “superconducting circuit” with a pair of loop shaped sensors. Interaction between the particles and the circuit only becomes appreciable if they get very near, or inside the loops. The circuit has two possible states denoted \(|\Phi_0\rangle\) and \(|\Phi_1\rangle\) with an energy gap \( \Delta \) between them and a free evolution determined by the pauli operator \( H_L = \frac{\Delta}{2} Z \), where \( Z = |\Phi_0\rangle\langle\Phi_0| - |\Phi_1\rangle\langle\Phi_1| \). Through the loops, the circuit is sensitive to the particles’ spins and is wired in such a way that when particle \( A \) enters the left loop and particle \( B \) enters the right loop the following operation is executed,

\[
|s\rangle|\Phi_0\rangle \rightarrow |s\rangle|\Phi_0\rangle \quad (4)
\]

\[
|t\rangle|\Phi_0\rangle \rightarrow |s\rangle|\Phi_1\rangle \quad (5)
\]

Such operation could be for example a SWAP gate on the \( \{|s\rangle|\Phi_0\rangle, |s\rangle|\Phi_1\rangle, |t\rangle|\Phi_0\rangle, |s\rangle|\Phi_1\rangle\} \) basis. Details on how such coupling between superconducting qubits and spins can be achieved are not important for our discussion, but can be found in [15]. We will refer to the circuit from now on as the loop or simply as the letter \( L \).

Now, suppose the environment decoheres the spin state of particles \( AB \) according to,

\[
|s\rangle_{AB}|0\rangle_E|\Phi_0\rangle_L \rightarrow \sqrt{1-p}|s\rangle_{AB}|0\rangle_E|\Phi_0\rangle_L + \frac{\sqrt{p}}{\sqrt{2}} \left( |\uparrow\rangle_A \downarrow_B |1\rangle_E + |\downarrow\rangle_A \uparrow_B |2\rangle_E \right) |\Phi_0\rangle_L
\]

\[
= \sqrt{1-p}|s\rangle_{AB}|0\rangle_E|\Phi_0\rangle_L + \frac{\sqrt{p}}{\sqrt{2}} \left( |\uparrow\rangle_A \downarrow_B |1\rangle_E + |\downarrow\rangle_A \uparrow_B |2\rangle_E \right) |\Phi_0\rangle_L
\]

(6)

where \(|0\rangle_E, |1\rangle_E, |2\rangle_E\) are orthogonal states of the environment, \( p \) is the probability of error and \(|\pm\rangle_E = (|1\rangle_E \pm |2\rangle_E)\). This channel can be seen as dephasing of a logical qubit spanned by the states defined as \(|\uparrow\rangle_{AB} = |0\rangle, |\downarrow\rangle_{AB} = |1\rangle\). We denote the dephasing superoperator acting on \( ABL \) as \( D \). Dephasing is one example of an environment. For a different example, dimer destruction by photodissociation, see the appendix. After application of \( D \) there is a non-vanishing probability that the particles \( AB \) are found in a triplet state. In that case the interaction energy \( V(R) \) between \( AB \) will change to a repulsive potential and cause the particles to push each other away and into the loops.

After a certain time-of-flight the particles reach the loops and the interaction between \( L \) and \( AB \) defined in Eqs. 4, 5 becomes important. At this point the relevant term in the wavefunction (6) proportional to \( \sqrt{p} \) evolves as

\[
\left( |s\rangle_{AB} |+\rangle_E |1\rangle_E L + |\rangle_E |\Phi_0\rangle_L \right) \frac{1}{\sqrt{2}}
\]

(7)
The particles $A$ and $B$ are corrected back to the singlet state, their mutual potential becomes once again attractive and they move towards each other and out of the loops. After a transient time, the orbital wavefunctions settle back in the equilibrium position of $V(R)$ for the molecular term $1\Sigma^+$ and the particles fall back in their initial singlet state. We can give an effective description of this dynamics in terms of a recovery superoperator acting on the joint system $ABL$. This recovery channel will be denoted $R$.

After one recovery the loop is entangled with the environment and has non-vanishing entropy. An external source of energy is required to “erase” the loop’s state and reset it to $|\Phi_0\rangle$, so that the whole process can start over. This erasing step requires a source of non-equilibrium and can happen stochastically. The non-equilibrium source could be a heat bath at a higher temperature, a strong magnetic field or any energetic resource floating around the environment. It is analogous to the sun in the case of photosynthesis or ATP for cell processes. Effectively we may describe this step by an appropriate amplitude damping channel we will refer to as the forgetness map $F$.

**MASTER EQUATION**

The behaviour of the qubit qualitatively described above is complex, certainly hard to predict algebraically and perhaps numerically challenging: it requires modelling involved stochastic quantum equations. It is expected however that general features of the system can be effectively captured by a markovian master equation describing a kind of continuous limit in which the recovery and forgetness jumps happen on a time scale much shorter than the time over which the qubot is observed. The system is then expected to behave as a continuous error correcting code like the one discussed in [46].

Dephasing $D$ competes with the recovery $R$ and forgetness $F$ and the joint $ABL$ density matrix $\rho \in \mathcal{B}(\mathcal{H}_{AB} \otimes \mathcal{H}_L)$ effectively evolves according to the master equation,

$$\dot{\rho} = -i[H, \rho] + D(\rho) + R(\rho) + F(\rho)$$ (8)

where $H = \mathbb{1} \otimes \frac{\Delta}{2}Z$ is the loop hamiltonian and the general Lindblad form $L(\rho)$ is given by

$$L(\rho) = \sum_a \left( L_a \rho L_a^\dagger - \frac{1}{2} L_a^\dagger L_a \rho - \rho \frac{1}{2} L_a^\dagger L_a \right)$$ (9)

with $L_a$ the quantum jump operators. Free hamiltonian evolution of the spins has been omitted for simplicity and we take $\hbar = 1$.

The system $AB$ is comprised of two qubits, but we are interested in the two dimensional subspace generated by the singlet and triplet states $\{ |s\rangle, |t\rangle \}$. We will thus treat $AB$ as a logical qubit. Recalling the definition of the computational basis $|\uparrow\downarrow\rangle_{AB} \equiv |\bar{0}\rangle, |\downarrow\uparrow\rangle_{AB} \equiv |\bar{1}\rangle$ given above, the quantum jump operators for the dephasing channel are

$$D_0 = \sqrt{\Gamma} |\bar{0}\rangle \langle \bar{0}| \otimes \mathbb{1}, \quad D_1 = \sqrt{\Gamma} |\bar{1}\rangle \langle \bar{1}| \otimes \mathbb{1},$$ (10)

where $\Gamma$ is the decoherence rate.

The channel $R$ is defined by the recovery operators

$$R_0 = \sqrt{r} |s\rangle \langle s| \otimes \mathbb{1}, \quad R_1 = \sqrt{r} |t\rangle \langle t| \otimes X$$ (11)

where $|s\rangle = (|\bar{0}\rangle - |\bar{1}\rangle) / \sqrt{2}$, $|t\rangle = (|\bar{0}\rangle + |\bar{1}\rangle) / \sqrt{2}$, $X = |\Phi_0\rangle \langle \Phi_1| + |\Phi_1\rangle \langle \Phi_0|$ is the bit-flip operator in the $\{ |\Phi_0\rangle, |\Phi_1\rangle \}$ basis and $r$ is the recovery rate. For our qubot, the recovery rate is bound by the inverse time necessary to complete one full recovery and return to the

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**FIG. 2:** (a) Transients of concurrence and entropy of $AB$ and entropy of loop as a function of time measured in units of the inverse loop energy $\hbar/\Delta$; rates for this plot are $\Gamma/\Delta = 1, \gamma/\Delta = r/\Delta = 1.5$. (b) Stabilization time as a function of forgetfulness rate.
initial state. We can then say that $r$ is roughly the inverse ‘recovery time’ given by

$$r \approx (t_c + \gamma^{-1})^{-1}$$ (12)

where $t_c$ is a correction time (that is the time needed for the particles $AB$ to reach the loop plus the time necessary for the $ABL$ interaction to occur) and $\gamma^{-1}$ the inverse forgetting rate, or the time needed for the loop to reset to state $|\Phi_0\rangle$. 

Finally, the $F$ superoperator consists in an amplitude damping channel and is hence given by the jump operator

$$F = \sqrt{\gamma} \mathbb{1} \otimes |\Phi_0\rangle\langle \Phi_1|.$$ (13)

We can numerically integrate the master equation for the initial state

$$\rho(0) = |s\rangle\langle s| \otimes |\Phi_0\rangle\langle \Phi_0|$$ (14)

and compute the concurrence $C(AB)$ and entropy $S(AB)$ of $AB$, and the entropy of the loop $S(L)$ as functions of normalized time $\Delta t$ (that is, time measured in units of the transition frequency $\Delta^{-1}$ between states of the loop) [17]. For comparison, we also calculate the concurrence of a pair of free spins initially in a singlet state under the influence of a dephasing channel with rate $\Gamma$. Since $r^{-1}$ is given by $\gamma^{-1}$ plus an additive constant $t_c$ defined solely by internal properties of the system, it is interesting to study the behavior of the qubit in terms of $\Gamma$ and $\gamma$. Hence we assume $t_c \ll \gamma^{-1}$, the rate of available resources is much shorter than the reaction rate of the system.

As we can see in Figure 2(a) the concurrence of a pair of free spins in a dephasing environment rapidly degrades to zero (blue curve). The qubit spins, on the other hand, decay to a mixed steady state with non-vanishing entanglement (orange curve). The dashed red and green curves show the qubit and loop von Neumann entropies, respectively. Initially zero, the entropies increase to a steady value. The levels of entanglement and entropy to which the system stabilizes and the necessary time for reaching stability are dependent on the decoherence $\Gamma$, recovery $r$ and forgetting $\gamma$ rates.

An interesting question is how long the device takes to reach the steady state. To quantify that, we define the stabilization time $t_o$ as the time at which the concurrence of $AB$ satisfies the condition

$$\frac{C_{t_o} - C_\infty}{C_\infty} < 0.1\%,$$ (15)

where $C_{t_o}$ is the concurrence at time $t_o$ and $C_\infty$ the concurrence at infinite time. Numerically, $C_\infty$ is reached when variations in the concurrence become of the order of the numerical precision. A plot of the stabilization time is shown in Figure 2(b) as a function of the recovery rate $\gamma/\Delta$ for four different decoherence rates. For smaller values of $\Gamma$ (weaker decoherence), small increases in $\gamma/\Delta$ make a large difference in the stabilization time $\Delta t_o$. As the decoherence rate assumes larger values (stronger decoherence), increasing $\gamma/\Delta$ becomes less effective.

Figure 3 shows the steady state values of concurrence and entropies for the qubit and loop as a function of the rates $\Gamma, \gamma$. The dashed line indicates the curve $\Gamma = 0.2\gamma$, clear from the bare plots of concurrence and entropy. Below this line $C(AB) \gtrsim 0.6$ and $S(AB), S(L) \lesssim 0.2$, indicating a considerable amount of entanglement and a low entropy. We thus numerically find that if the decoherence and recovery rates satisfy

$$\gamma > 5\Gamma$$ (16)

the qubit is able to significantly protect its e-bit. Erasing the loop state back to $|\Phi_0\rangle$ is an operation which takes at least a time $t_{\text{erase}} \approx \Delta^{-1}$ [15]. Hence, the maximum forgetfulness rate is expected to be $\gamma_{\text{max}} \approx \Delta$. In combination with [16] we then get that a successful qubot satisfies $\Delta \gtrsim 3\Gamma$.
DISCUSSION

A common feature of living organisms is employing different molecular conformations to manipulate a potential barrier and execute a function. Na, K ATPase ion pumps provide an interesting example in which conformations alter the potential landscape seen by an ion and consequently transport it in a preferred direction \[3, 4\]. Our qubot example operates in a similar way exploiting interatomic potential changes and moving parts to “proofread” and protect quantum information, consequently sustaining a preferred quantum state.

In the future, nano-mechanical designs with moving parts could be built using single atom tweezers \[50, 51\] and the available ultracold molecule toolbox \[52, 53\]. Trapped ions \[54\], NV-centers \[55\] and levitated nano-particles \[56, 57\] can also couple internal and motional degrees of freedom to superconducting circuits, and similar mechanisms can be envisioned. One can also imagine qubits with no moving parts where quantum errors induce a potential change which triggers a recovery operation involving only internal states of the system. For instance, a spin-ensemble quantum memory of NV-center defects in diamond glued on top of a superconducting circuit can collectively couple to a qubit \[50\]. This could be exploited to create a self-error correcting system capable of protecting quantum data stored in the spins.

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Appendix: an alternative environment

In the main text we have considered the dephasing environment which “learns” with a certain probability the spin states of particles $AB$ thus causing decoherence of the e-bit. We might consider different environments. A case of interest for ultracold quantum chemistry experiments is “dimer destruction by a diode laser” as studied in [1]. A molecule is formed by particles $AB$, bound in the $^1\Sigma^+$ molecular term. A laser shining at the molecule may induce a transition to an excited state, and subsequent decay to either the $^1\Sigma^+$ or $^3\Sigma^+$ states. When the system decays to the $^3\Sigma^+$ state, the potential between $AB$ changes to repulsive, and the molecule is destroyed. This is called photodissociation and a schematic representation of the process is shown in Figure S1(a). In this situation the spins are still in a triplet entangled state after the molecule has dissociated, however, the particles will fly apart and the e-bit will be delocalized and possibly lost in practice.

The “photodissociation environment” $\mathcal{P}$ given by the laser acts as

$$|s\rangle_{AB}|0\rangle_E|\Phi_0\rangle_L \rightarrow \sqrt{1-p}|s\rangle_{AB}|0\rangle_E|\Phi_0\rangle_L + \sqrt{p}|t\rangle_{AB}|1\rangle_E|\Phi_0\rangle_L$$

(S1)

where $p$ is the probability of error and $|0\rangle_E, |1\rangle_E$ are orthogonal states of the environment. The qubot corrects this state to

$$|s\rangle_{AB} \otimes (\sqrt{1-p}|0\rangle_E|\Phi_0\rangle_L + \sqrt{p}|1\rangle_E|\Phi_1\rangle_L)$$

(S2)

thus entangling the loop to the environment. The forgetness map then erases the loop memory and the process restarts.

If the molecule transitions to the triplet state, dissociation prevents the system from going back to the singlet configuration. We can describe this process as a decay from $|s\rangle$ to $|t\rangle$. The corresponding quantum jump operator is $P = \sqrt{\Gamma}|t\rangle\langle s| \otimes 1$. We numerically solve the master equation presented in the main text, with the superoperator $\mathcal{P}$ replacing $\mathcal{D}$. Figure S1(b) shows the fidelity between the original singled spin state and the time-dependent state under the action of photodissociation for free spins (blue curve) and the qubot (orange curve).

![FIG. S1: (a) Schematic representation of the dissociation process. (b) Time-dependent fidelity with respect to singlet; rates for this plot are $\Gamma/\Delta = 1, \gamma/\Delta = r/\Delta = 1.5$.](image)

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