Quantum Simulator of an Open Quantum System Using Superconducting Qubits: Exciton Transport in Photosynthetic Complexes

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Quantum simulator of an open quantum system using superconducting qubits: exciton transport in photosynthetic complexes

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Open quantum system approaches are widely used in the description of physical, chemical and biological systems. A famous example is electronic excitation transfer in the initial stage of photosynthesis, where harvested energy is transferred with remarkably high efficiency to a reaction center. This transport is affected by the motion of a structured vibrational environment, which makes simulations on a classical computer very demanding. Here we propose an analog quantum simulator of complex open system dynamics with a precisely engineered quantum environment. Our setup is based on superconducting circuits, a well established technology. As an example, we demonstrate that it is feasible to simulate exciton transport in the Fenna-Matthews-Olson photosynthetic complex. Our approach allows for a controllable single-molecule simulation and the investigation of energy transfer pathways as well as non-Markovian noise-correlation effects.

Understanding strongly interacting quantum systems with many degrees of freedom is one of the big challenges in physics and chemistry. Classical computational methods are restricted by exponentially increasing amount of resources required for the simulations. Quantum computers are conjectured to be a possible solution as the resources to simulate arbitrary quantum systems grow polynomially with the size of the system under study. However, universal quantum computers of sufficient size and performance are not available yet, one of the big problems being the loss of quantum mechanical coherence, i.e., decoherence. Designing a special quantum system in the laboratory, which mimics the quantum dynamics of a particular model of interest, see for example, Refs. [2, 3], can be a more viable alternative to an all-purpose quantum computer.

Here we propose a quantum simulator architecture using superconducting quantum bits (qubits) that is capable of simulating complex open quantum systems using currently-available technology in realizable parameter ranges. We will focus on the Fenna-Matthews-Olson (FMO) pigment-protein complex on a single molecule level. The recent observations [11, 12] of quantum beatings and long-lived quantum coherence in several photosynthetic light-harvesting complexes, such as the FMO complex in the green sulfur bacterium Chlorobium tepidum or the reaction center of the purple bacterium Rhodobacter sphaeroides, suggest possible evidence that quantum effects give rise to the high energy transport efficiency found for these complexes. There is a remarkable amount of recent theoretical research related to the question of the molecular structure, vibrational environment, the origin and the role of long-lived quantum coherences [13, 23]. The electronic degrees of freedom are coupled to a finite temperature vibrational environment and the dynamics of the relevant electronic system can be studied by means of open quantum system approaches. In classical computing, the focus of much of the research has been on reducing the magnitude and influence of environmental decoherence and dissipation. However, controlled coupling to a dissipative environment can also be exploited [24, 26]. In this work, we focus on engineering the decoherence to simulate open quantum systems that are challenging to study using classical computers.

We propose two approaches for simulating the vibrational environment. The first approach is based on engineering a classical noise source such that it represents the atomistic fluctuations of the protein environment. A prototypical experiment of environment-assisted quantum transport (ENAQT) can be performed [16]. The second approach allows for the precise engineering of the complex non-Markovian environment, i.e., an environment that has long-term memory. This is achieved by the explicit coupling of quantum inductor-resistor-capacitor (LRC) oscillators to the qubits which allows for energy and coherence exchange between the resonators and the qubits. Both approaches are based on present-day superconducting qubit implementations. Fabrication of superconducting circuitry is done by several research labs. We focus here on flux qubits, where two-qubit coupling was shown to be sign- and magnitude-tunable [27, 28] and methods of scaling to a moderate number of qubits have been discussed in Refs. [24, 30]. We show that realistic simulation of photosynthetic energy transfer is feasible with current superconducting circuit devices.

I. THE MODEL HAMILTONIAN

We are interested in the dynamics of a finite dimensional system which is linearly coupled to a bath of harmonic oscillators. In the following we refer to the system as “electronic system” and to the quantum environment as “phonon bath” or “vibrational environment”. The
corresponding total Hamiltonian is written as

\[ H_{\text{tot}} = H_{\text{el}} + H_{\text{ph}} + H_{\text{el-ph}}. \]  

(1)

A. The system

We are often (e.g., in the FMO complex) interested in the transfer of a single electronic excitation. Thus basis states \(|j\rangle\) are defined by the electronic excitation residing on molecule (site) \(j\) and all other sites being in their electronic ground state. The electronic Hamiltonian in this site basis is given by

\[ H_{\text{el}} = \sum_{j=1}^{N} \varepsilon_j |j\rangle \langle j| + \sum_{i<j} V_{ij} (|i\rangle \langle j| + |j\rangle \langle i|), \]

(2)

The diagonal energies \(\varepsilon_j\) are identified with the electronic transition energies of site \(j\) and the off-diagonal elements \(V_{ij}\) are the intermolecular (transition-dipole-dipole) couplings between sites \(i\) and \(j\). Different local electrostatic fields of the protein at different sites shift the electronic transition energies \([15]\), resulting in a complicated energy landscape.

B. Coupling to the quantum environment

The vibrational environment is represented by a set of displaced harmonic oscillators. The Hamiltonian of the phonon bath is written as \(H_{\text{ph}} = \sum_{j=1}^{N} H_{\text{ph}}^j\), where

\[ H_{\text{ph}}^j = \frac{1}{2} \sum_{\ell} \hbar \omega_{j\ell}^2 (a_{\ell j}^\dagger a_{\ell j}^\dagger + a_{\ell j} a_{\ell j}) \]

and \(a_{\ell j}^\dagger\) (\(a_{\ell j}\)) being the creation (annihilation) operator of excitations in the \(\ell\)-th bath mode of site \(j\). In the present work we restrict to the situation where each site has its own phonon environment which is uncorrelated with the phonon modes at the other sites. This is motivated by recent results obtained for the FMO complex \([32, 33]\). The diagonal part of the electronic Hamiltonian couples linearly to the phonon modes. The electron-phonon coupling term can be written as

\[ H_{\text{el-ph}} = \sum_{j=1}^{N} H_{\text{el-ph}}^j = \sum_{j=1}^{N} |j\rangle \langle j| \left( \sum_{\ell} \chi_{j\ell} (a_{\ell j}^\dagger + a_{\ell j}) \right). \]

(3)

Here \(\chi_{j\ell} = \hbar \omega_{j\ell}^2 d_{j\ell}\) is the coupling between the \(j\)-th site and the \(\ell\)-th phonon mode with \(\omega_{j\ell}\) being the frequency of the \(\ell\)-th phonon mode coupled to the \(j\)-th site and \(d_{j\ell}\) is the dimensionless displacement of the minima of the ground and excited state potentials of the \(\ell\)-th phonon mode at site \(j\). Notice that the so-called reorganization energy \(\lambda_j = \sum_{\ell} \hbar \omega_{j\ell}^2 d_{j\ell}^2 / 2\) was implicitly included in the above electronic transition energy \(\varepsilon_j\), with \(\varepsilon_j\) being the energy difference of the minima of the potential energy surfaces for site \(j\), see Figure 1 (a) and the Supporting Information for more details.

It is known that complete information about the effect of the environment on a quantum system is determined by the spectral density (SD) function \([34]\), which is defined by

\[ J_j(\omega) = \sum_{\ell} |\chi_{j\ell}|^2 \delta(\omega - \omega_{j\ell}) \]

(3)

for site \(j\). Due to the high number of modes of the environment, \(J_j(\omega)\) can be considered as a continuous function of \(\omega\). To account for finite temperature, we transform the spectral density \([35, 36]\). The new function \(C_j(\omega, T)\) fulfills the detailed balance condition \([33]\) and we name it “temperature-dependent spectral density”.

It turns out that the relevant spectral densities of our problem can be approximated by a finite number of broadened peaks. These broadened peaks can often be associated with the vibrational modes of the molecules. Upon electronic excitation of a molecule, the vibronic Gaussian wavepacket of the ground state is projected into a displaced wavepacket in the excited state at the Franck-Condon point, see Figure 1 (a). The nuclei wavepacket then moves on the excited state potential energy surface and reorganizes to the minimum point while the reorganization energies of the respective modes are dissipated.

Finally, to facilitate the comparison with flux qubits...
we rewrite the total Hamiltonian \[ H_{\text{tot}} \] using Pauli matrices

\[
H_{\text{tot}} = \frac{1}{2} \sum_{j=1}^{N} \tilde{\varepsilon}_j \sigma_z^j + \frac{1}{2} \sum_{i<j}^{N} V_{ij}(\sigma_x^i \sigma_x^j + \sigma_y^i \sigma_y^j) + \sum_{j=1}^{N} \hbar \omega_{\ell_j} \left( a_{\ell_j}^\dagger a_{\ell_j} + \frac{1}{2} \right) + \sum_{j=1}^{N} \chi_{j\ell} \sigma_z^j \left( a_{\ell_j}^\dagger + a_{\ell_j}^\dagger \right).
\]

Expressing the above Hamiltonian in the system energy eigenbasis, defined by \( H_{\text{tot}} | M \rangle = E_M | M \rangle \), we have

\[
H_{\text{tot}} = \sum_M E_M | M \rangle \langle M | + \sum_{M,N,\ell} \mathcal{X}_{MN}^\ell | M \rangle \langle N | (a_{\ell}^\dagger + a_{\ell}^\dagger) + H_{\text{ph}} \text{ with } \mathcal{X}_{MN}^\ell = \sum_j \langle M | j \rangle \langle j | N \rangle \chi_{j\ell}. \]

This shows that the system-bath coupling is off-diagonal in the eigenbasis.

C. The classical noise approximation

Although the main goal of the present paper is to simulate the fully quantum mechanical Hamiltonian \[ H_{\text{tot}} \] it is also useful to consider the much simpler (but important) case where the quantum environment is replaced by time-dependent fluctuations of the transition energies. This is the basis of the often employed Haken-Strobl-Reineker (HSR) model for excitation transfer \[ 37 \]. Furthermore, atomistic MD/QM/MM simulations \[ 32, 33 \] can readily provide noise time-series. In the classical noise approach, the system dynamics is obtained by averaging over many trajectories with the time-dependent Hamiltonian

\[
\tilde{H}_{\text{tot}} = \frac{1}{2} \sum_{j=1}^{N} [\tilde{\varepsilon}_j + \delta \tilde{\varepsilon}_j(t)] \sigma_z^j + \frac{1}{2} \sum_{i<j}^{N} V_{ij}(\sigma_x^i \sigma_x^j + \sigma_y^i \sigma_y^j),
\]

where the influence of the environment is solely contained in the time-dependent site energy fluctuations \( \delta \tilde{\varepsilon}_j(t) \). Often, as in the HSR model, it is assumed that the fluctuations are uncorrelated Gaussian white noise.

II. THE FMO COMPLEX

The model Hamiltonian \[ H_{\text{tot}} \] can be used to describe a single excitation in the FMO complex. The FMO complex acts as a highly efficient excitation wire, transferring the energy harvested by the photosynthetic antennae to a reaction center. The FMO trimer has a trimeric structure exhibiting C_{3v} symmetry and each of the monomers consists of a network of eight \[ 23 \] bacteriochlorophyll a (BChl a) pigment molecules. Since the coupling between monomers is very small and can be neglected on the time-scales of interest, we focus on a single monomer in the following. The BChl pigments in the monomer are surrounded by a protein environment. Conformational motions of this protein environment (static disorder) are slow compared to the timescale of interest and affect energy levels of the pigments by electrostatic interaction \[ 15 \]. The ranges of site energy differences \( |\tilde{\varepsilon}_i - \tilde{\varepsilon}_j| \) and couplings \( V_{ij} \) are given in table I. These parameters lead to the energy spectrum of the FMO monomer given in Figure I (b).

In the present work, we consider two spectral densities relevant to the FMO complex. First, a model super-Ohmic SD \[ 14 \], \( J(\omega) = \lambda/\omega_0 \frac{\omega}{\omega} \), with reorganization energy \( \lambda = 35 \text{ cm}^{-1} \) and cutoff frequency \( \omega_0 = 150 \text{ cm}^{-1} \), shown as the transformed \( C(\omega, T) \) by the blue dashed line in Figure I (a). The electronic excitations of several delocalized exciton states.

III. THE SIMULATOR

It is challenging to simulate the open quantum system described in the previous sections on conventional computers \[ 20, 36, 39 \], even using modern parallel processing units \[ 40, 42 \]. Here we propose using flux qubits coupled with tunable flux-flux couplings for this task. The environment is modeled by classical noise or quantum oscillators coupled to the flux qubits.

A. The system Hamiltonian

Consider first a single flux qubit. The relevant quantum states are the ones with magnetic flux pointing up \( |\uparrow\rangle \) and down \( |\downarrow\rangle \) or, equivalently, opposite directions of persistent current along the loop. In this bare basis, the Hamiltonian of a flux qubit is given by

\[ H = (\mathcal{D} \sigma_z + \Delta \sigma_x)/2, \]

where \( \mathcal{D} \) is the energy bias between \( |\uparrow\rangle \) and \( |\downarrow\rangle \) and \( \Delta \) is the tunnel splitting between the two states. Here \( \mathcal{D} = 2I_p(\phi_x - \phi_y)/2 \) \[ 13 \] with \( I_p \) being the persistent current of the qubit and \( \phi_0 = h/2e \) being the flux quantum. \( \mathcal{D} \) can be tuned to zero to neglect the \( \mathcal{D} \sigma_z \) term.
A tunable transverse interaction between flux qubits equivalent to that in $H_{\text{cl}}$ can be realized using additional ‘coupler’ qubits [27, 44]. A schematic of such a simulator is given in Figure 2 (a). The Hamiltonian of the coupled qubit system can be written as $H_q = \sum_{j=1}^{N} \Delta_j \sigma_j^z/2 + \sum_{i<j} g_{ij}(\Delta_{ij}) \sigma_i^x \sigma_j^x$ with $g_{ij}(\Delta_{ij})$ being the coupling strength between flux qubits $i$ and $j$, which is given by $g_{ij}(\Delta_{ij}) \approx \mathcal{J}_{ij} - 2 \mathcal{J}_{ic} \mathcal{J}_{jc} / \delta_{ij}$, where $\Delta_{ij}$ is the (tunable) tunnel splitting of the coupler qubit and we have defined $\delta_{ij} \equiv \Delta_{ij}^c - (\Delta_i + \Delta_j) / 2$ and $\mathcal{J}_{mn} \equiv \mathcal{M}_{mn} \mathcal{I}_{j} \mathcal{I}_{j}^c$ with $m,n \in i,j,c$ [44]. Here, $\mathcal{M}_{mn}$ is the mutual inductance between qubits $m$ and $n$. This expression is valid to leading order when $\delta_{ij} \gg |\Delta_i - \Delta_j|, \mathcal{J}_{ic}, \mathcal{J}_{jc}$. Notice that by choosing the magnitude of $\Delta_{ij}^c$ to be smaller or larger than $(\Delta_i + \Delta_j) / 2$ we can change the sign of the effective coupling. Rewriting the above Hamiltonian in the energy eigenbasis of the qubit $|\pm\rangle = (|\uparrow\rangle + |\downarrow\rangle) / \sqrt{2}$ converts $\sigma_z^i \rightarrow \sigma_+^i$ and $\sigma_z^i \sigma_z^i \rightarrow \sigma_+^i \sigma_+^i \approx (\sigma_+^i \sigma_+^i + \sigma_-^i \sigma_-^i) / 2$ in the rotating wave approximation (neglecting strongly off-resonant couplings). This results in

$$H_q \approx \frac{1}{2} \sum_{j=1}^{N} \Delta_j \sigma_j^z + \frac{1}{2} \sum_{i<j} g_{ij}(\Delta_{ij}) \left( \sigma_j^+ \sigma_j^z + \sigma_j^z \sigma_j^+ \right),$$

which is of exactly the same form as the system part (first line) of Eq. 4 with $\Delta_j$ and $g_{ij}(\Delta_{ij})$ corresponding to $\tilde{\varepsilon}_j$ and $V_{ij}$, respectively. It is advantageous for the experimental implementation to note that the dynamics of Eqs. 4 and 6 does not depend on absolute site energies $\tilde{\varepsilon}_j$ and $\Delta_j$, but only on energy differences $|\tilde{\varepsilon}_i - \tilde{\varepsilon}_j|$ and $|\Delta_i - \Delta_j|$, respectively.

![FIG. 2. Circuit diagram of the proposed quantum simulator. (a) The qubit states are encoded in the quantized circulating current of the qubit loop. The red crosses denote Josephson junctions. Two flux qubits are coupled with a tunable $\sigma_x \sigma_i \sigma_z$-coupling. Each of the qubits is independently coupled to a finite number of quantum LRC oscillators to simulate the non-Markovian vibrational environment. (b) Simulating the vibrational environment by adding a classical noise to each qubit.](image)

![FIG. 3. Experimental layout for simulating the exciton dynamics and environment assisted quantum transport (ENAQT) in the FMO complex (the architecture is based on the interactions given in Ref. [23], where for simplicity of the graphic the couplings below 15 cm$^{-1}$ are not shown). $Q_j$ represent single flux qubits. To simulate a biologically relevant case, one of these qubits, $Q_3$ shown in green, is prepared initially in the excited state while the others are set to the ground state. The measurement is performed on the target site, $Q_1$ shown in red. Sinks can be used to trap the energy and quantify the transfer efficiency.](image)
see Figure 2 (b). Such a noise affects the tunnel splitting $\Delta_j$ in the qubit Hamiltonian. On one hand, the noise can be actively created and send to the qubit by a time-dependent voltage $\tilde{V}$ applied to a control loop \[10\]. Regarding the passive approach, an environmental loop exhibits standard Johnson-Nyquist noise \[47\]. The bath spectrum $J(\omega)$ of the noise seen by the qubit can be related to the real part of the impedance $Z(\omega)$ \[48\]: $J(\omega) = K \omega \Re\{Z(\omega)\}$, with $K$ being a constant depending on the self-inductance of the environment loop and its coupling strength to the flux qubit. With classical circuit design $Z(\omega)$ can be tailored to produce the desired frequency dependence, for example, the ones in Refs. \[13\] \[14\] \[20\].

With simple classical noise a prototypical experiment of ENAQT can be performed \[16\], see Figure 3. In the FMO complex, the initial state of the simulation can be one of the sites $Q_1$, $Q_6$, or $Q_8$ which are close to the antenna in the biological system. Measurement of success of the transport is performed at site $Q_3$ or by evaluating the population lost to the sink. Such an experiment can show that the environment is not always adversarial, but instead can make certain processes, like quantum transport, more efficient (see the Supporting Information for more details). This transport efficiency should exhibit a maximum at a dephasing rate that corresponds to room temperature in the biological system \[10\]. Similar ideas of simulating ENAQT have been pursued in \[49\] \[50\].

C. Non-Markovian approach

In order to simulate the complex environment described by Eq. 4 and capture the non-Markovian effects, we propose to couple each of the flux qubits inductively to an independent set of a few damped quantum LRC oscillators, see Figure 2 (a). The coupling Hamiltonian between the qubits and oscillators \[51\] in the energy eigenbasis is given by $H_{\eta-osc} = \sum_{j=1}^{N_{LRC}} \sum_k \eta_{jk} \sigma_z^{jk} (b_k^\dagger + b_k)$, with $b_k^\dagger$ ($b_k$) being the creation (annihilation) operator of the $k$-th oscillator in site $j$. The coupling strength is given by $\eta_{jk} \equiv \mathcal{M}_{jk} I_0^k (d\Delta_j/d\Phi_k^j)$, where $I_0^k$ is the root mean square (RMS) amplitude of the current in the $k$-th oscillator ground state.

To simulate the original spectral density \[3\] we have to design the frequencies and couplings of the oscillators in such a way that the spectral density is reproduced up to a global scaling factor. From the implementation point of view, we are limited to a finite number of oscillators. Thus, we decompose the spectral density of interest into a moderate number of spectral densities of damped oscillators. The spectral density of a single oscillator coupled to a flux qubit can be derived by using a quantum Langevin equation approach \[52\] \[53\] and following the detailed balance condition \[35\].

$$C_{osc}(\omega, T) = \mathcal{D} \left[ \frac{e^{\hbar \omega/k_B T}}{\kappa^2 + 4(\omega - 2\pi \omega_0)^2} + \frac{1}{\kappa^2 + 4(\omega + 2\pi \omega_0)^2} \right]$$

where $\mathcal{D} = (\sqrt{8/\pi} \kappa \eta^2) / (e^{\hbar \omega_0/k_B T} + 1)$ with $\omega_0$ being the transition frequency of the oscillator and $\eta$ being the coupling strength of the oscillator to the flux qubit. Here, $\kappa = \kappa_0 \exp(-|\omega|/\alpha) \omega^2/\omega_0^2$ with $\kappa_0$ being the damping rate and $\alpha$ being a free parameter chosen reasonably to get the desired spectral density. By knowing the above spectral density for the damped quantum oscillators, we first simulate the temperature-dependent super-Ohmic spectral density. At 300 K this spectral density can be simulated with a set of 6 LRC oscillators coupled to each of the flux qubits, see Figure 4 (a), and at 77 K it can be simulated with a set of 7 oscillators (see Figure S1 (a) in the Supporting Information). For the experimental spectral density, we need to couple, for example, 15 oscillators to each qubit, see Figure 2 (b). Notice that the so-obtained SDs in Figure 4 are highly accurate and we can use fewer coupled oscillators if we are interested in less details of the spectral densities. The coupling of the oscillators to the flux qubit results in an additional shift of the qubit tunnel splitting $\Delta_j$ due to the reorganiza-
tion energy of the oscillators. This has to be taken into account in the design of the circuit energy landscape.

IV. EXPERIMENTAL FEASIBILITY

The simulation of the time evolution of the FMO complex requires a moderately coherent eight-qubit system, which would be realizable using the flux qubits demonstrated in Ref. [28] and the coupling geometries and methods of Refs. [27, 44]. In the FMO complex the site energies/chlorophyll excitation energies are around 12500 cm$^{-1}$, with the average site-dependent static shifts of the order of 250 cm$^{-1}$. We emphasize again that only the site-energy differences, not the site energies themselves, play a role in the single-exciton dynamics. The magnitudes of the coupling strengths between the chlorophyll molecules are smaller than 120 cm$^{-1}$ [14]. For superconducting flux qubits, implementable range of the tunnel bias $\Delta_j$ is in the range of approximately zero to 13 GHz [28], while the coupling strengths $g_{ij}$ were measured in the range of one GHz to approximately zero [27].

The parameters of the proposed quantum simulator are scaled through the time scale of quantum beatings ($\tau_{osc}$) to be consistent internally as well as with the implementation restrictions, see Table I. Photosynthesis occurs at ambient temperatures, e.g., 300 K, which then maps to 60 mK in superconducting-circuit experiments. The FMO dynamics is usually considered for up to 5 ps, which translates to the timescale of 25 ns in the flux qubits. The energy relaxation time ($T_1$) of a single qubit has been found [13, 54] to be on the order of a few $\mu$s, being a few orders of magnitude larger than the required exciton transfer time. Several coherent beatings between two coupled qubits have been observed [27]. Table II represents the summary of the required range of parameters for the superconducting simulator to imitate the dynamics of the FMO complex.

In simulating the quantum environment of the FMO complex, the required transition frequency of the LRC oscillators are in the range of 120 MHz to 3 GHz and the coupling to the qubits are around 8 MHz to 100 MHz, see Tables S2 and S3 in the Supporting Information. These parameters are experimentally reasonable. The geometry of Figure 3 may cause space problems in implementing this system. To avoid this, the parallel combination of resonators used to implement the desired spectral density can be mapped, for example, to a linear chain of oscillators [53, 57], such that only a single resonator would need to be coupled directly to each qubit, see Figure S2 in the Supporting Information. The quality factor (transition frequency/bandwidth) of the quantum oscillators in our proposed simulator are up to 50 or less (i.e., each of the oscillators is strongly overcoupled to an output 50 Ohm line). The coupling to the output line can be tunable to adjust the quality factor of each oscillator in situ. Finally, low-frequency flux noise ($1/f$ noise) is one of the decoherence sources in flux qubits. In our proposal, this noise is suppressed at the optimal working point [58], where $\varepsilon = 0$. All of the above numbers and observations suggest that the site energy differences to coupling ratios of the FMO complex as well as corresponding temperature and environmental couplings are achievable with superconducting circuits.

V. CONCLUSION

We have demonstrated that an appropriately designed network of superconducting qubit-resonator design can simulate not only the coherent exciton transport in photosynthetic complexes, but also the effect of a complicated quantum environment. We have highlighted its experimental feasibility with present-day technology. In particular, we have shown that a straightforward combination of superconducting qubits (representing the chlorophyll molecules) and resonators (simulating the phonon environment) can be used to obtain a reasonable approximation to the exciton and phonon degrees of freedom in the FMO complex. For example, we show ways to engineer a spectral density that reproduces the one of the biological system. One of the advantages of our proposed quantum simulator, compared to the computational methods, is simulating both diagonal and off-diagonal noise. Because of the additional complexity of considering the off-diagonal noise most of the non-Markovian computational methods only take the diagonal noise into the account. Another advantage is that, by design, we have a single molecule setup while all the ultrafast experiments use an ensemble of light harvesting complexes. This allows for more detailed studies of non-Markovian energy transfer pathways.

An important feature of our proposal is the potential to achieve a high level of environment engineering, in such a way that external noise is used to benefit the quantum coherent energy transfer process inside the molecule. However, the broader scope of our work is along the lines of biomimesis: the artificial recreation of biological processes, which are already highly optimized through evolution.

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ions, interpretations, recommendations and conclusions under Air Force Contract No. FA8721-05-C-0002. Opinion, laboratory is sponsored by the United States Air Force and S3 in the Supporting Information. Notice that the decay time in a single qubit (T1) does not need to be mapped directly from the FMO dynamics. With nowadays achievable decay times in superconducting qubits, which are 3 orders of magnitude larger than the excitation transfer time between the qubits, the dynamics of the FMO complex can be simulated.

TABLE I. Comparison of parameters for the FMO complex and the quantum simulator. The timescales shown below are for the dressed states of flux qubits coupled to the quantum harmonic oscillators. For more details see Figure S3 and Tables S1, S2, and S3 in the Supporting Information. Notice that the decay time in a single qubit (T1) does not need to be mapped directly from the FMO dynamics. With nowadays achievable decay times in superconducting qubits, which are 3 orders of magnitude larger than the excitation transfer time between the qubits, the dynamics of the FMO complex can be simulated.

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<th>Parameter</th>
<th>FMO model</th>
<th>Quantum simulator</th>
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<td>decay time (T1)</td>
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<td>average exciton transfer time</td>
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<td>temperature</td>
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I. SUPPORTING INFORMATION

II. COORDINATE REPRESENTATION OF THE MODEL HAMILTONIAN

In this section we derive the model Hamiltonian of a single molecule (Eq. [1] in the main article for \( N = 1 \)) from the Born-Oppenheimer approximation. Restricting to two electronic states, the ground state \(|g\rangle\) and the excited state \(|e\rangle\), the Hamiltonian in the Born-Oppenheimer approximation is [1]:

\[
H = H_{\text{nuc},g}(R)|g\rangle\langle g| + H_{\text{nuc},e}(R)|e\rangle\langle e|,
\]

where \( R \) describes the collection of \( 3N_{\text{nuc}} \) modes relevant to the molecule (both local and protein modes), \( R = \{ R_1, \ldots, R_{3N_{\text{nuc}}} \} \), with \( N_{\text{nuc}} \) being the number of nuclei. The Hamiltonians \( H_{\text{nuc},g/e}(R) \) describe the kinetic and potential energy of the nuclei, \( T_{\text{nuc}} \) and \( V_{\text{nuc}} \), respectively: \( H_{\text{nuc},g/e}(R) = T_{\text{nuc}} + V_{\text{nuc},g/e}(R) \). The potential energy is given by \( V_{\text{nuc},g/e}(R) = V_{\text{nuc}-\text{nuc}}(R) + E_{g/e}(R) \) with the inter-nuclear potential energy \( V_{\text{nuc}-\text{nuc}} \) and the potential energy due to the electrons \( E_{g/e}(R) \). We assume a displaced harmonic oscillator model for the potential of ground and excited state:

\[
V_{\text{nuc},g}(q) = U_g + \sum_{i=1}^{3N_{\text{nuc}}} \frac{\hbar \omega_i}{2} q_i^2,
\]

\[
V_{\text{nuc},e}(q) = U_e + \sum_{i=1}^{3N_{\text{nuc}}} \frac{\hbar \omega_i}{2} (q_i - d_i)^2.
\]

Here, we introduced the renormalized coordinates \( q = R - R_0 \), where \( R_0 \) are the equilibrium positions in the electronic ground state (minimum of the ground state potential energy surface). The respective energies of the electronic states at the minimum of the respective potentials are \( U_g \) and \( U_e \). We have assumed that the frequency \( \omega_i \) of mode \( i \) remains unchanged in the exited state. The displacement of the \( i \)th mode in the excited state is given by \( d_i \). The \( q \)-dependent energy gap is given by the difference of the two potentials:

\[
V_{\text{nuc},e}(q) - V_{\text{nuc},g}(q) = \Delta U + \sum_{i=1}^{3N_{\text{nuc}}} \frac{\hbar \omega_i}{2} q_i^2 - \sum_{i=1}^{3N_{\text{nuc}}} \hbar \omega_i d_i q_i,
\]

where the first term \( \Delta U = U_e - U_g \) is the energy difference between the potential minima of ground and excited state. The second term gives the reorganization energy:

\[
\lambda = \sum_i \lambda_i = \sum_i \frac{\hbar \omega_i}{2} d_i^2.
\]

The third term gives the linear dependence of the gap on the coordinates of the harmonic oscillator, and is the exciton-vibrational coupling term. The total Hamiltonian in the harmonic approximation is thus:

\[
H_{\text{tot}} = \left( \Delta U + \sum_i \lambda_i \right) |e\rangle\langle e| + \sum_i \frac{\hbar \omega_i}{2} q_i^2 + \sum_i \hbar \omega_i d_i q_i |e\rangle\langle e|.
\]

Here we defined the respective Hamiltonians for the electronic system, phonon bath and electron-phonon coupling, \( H_{el} \), \( H_{\text{ph}} \), and \( H_{el-\text{ph}} \). The system identity operator is given by \( 1 = |g\rangle\langle g| + |e\rangle\langle e| \).
III. ENERGY TRANSFER PATHWAYS FOR THE FMO COMPLEX

We briefly explain the red arrows in Figure 1 (b), which show schematically the downwards energy transfer pathways for the FMO complex, similar to Ref. [4] which considered seven-site model for the FMO complex.

From a system-bath model like Eq. (1) (main article), one can derive a master equation for the density matrix by using, for example, Redfield theory with the secular approximation [3]. Redfield theory assumes weak coupling and a Markovian bath. This leads to decoherence rates in the energy basis between energy states $M$ and $N$ given by $\frac{\hbar}{\sqrt{\Lambda}}$ (without loss of generality $\hbar \omega_{MN} = E_M - E_N > 0$):

\[
\Gamma_{MN}^\uparrow = 2\pi \gamma_{MN} J(\omega_{MN}) n(\omega_{MN}) ,
\]
\[
\Gamma_{MN}^\downarrow = 2\pi \gamma_{MN} J(\omega_{MN}) [n(\omega_{MN}) + 1] .
\]

Here, $\Gamma_{MN}^\uparrow$ ($\Gamma_{MN}^\downarrow$) is the rate up (down) in energy and $n(\omega_{MN})$ is the mean number of vibrational quanta with energy $\hbar \omega_{MN}$ that are excited at a given temperature $T$:

\[
n(\omega_{MN}) = 1/\left[ \exp(\hbar \omega_{MN}/k_B T) - 1 \right].
\]

The factor $\gamma_{MN} = \sum_j |\langle M|j\rangle|^2|\langle j|N\rangle|^2$ arises from the basis transformation between site and energy basis. In Figure 1 (a), the red arrows show a selected number of downward transitions with $\gamma_{MN} J(\omega_{MN}) \geq 0.3 \text{ cm}^{-1}$.

IV. ENVIRONMENT-ASSISTED QUANTUM TRANSPORT

Here we briefly discuss the main features of environment-assisted quantum transport and what is to be expected from an experiment scanning the ratio of dephasing rate over system energy scale. For the qubit system in our proposed quantum simulator, the couplings and the differences in the qubit splittings give a general energy scale $\Lambda$. The site energy level fluctuations lead to pure dephasing as the dominant decoherence mechanism, which is phenomenologically characterized by a pure dephasing rate $\gamma$. In the active noise engineering case, each site is driven, for example, by white noise with an amplitude $\sqrt{\gamma}$. The amplitude can be easily tuned in the external noise generator. In the passive case, the noise level can be regulated by the temperature of the sample. For both cases, if the dephasing rate $\gamma$ is much smaller than the energy scale $\Lambda$, quantum localization is predicted to arise from the disorder in the energy levels. This leads to a small population at the target site. Increasing the dephasing rate such that $\gamma \approx \Lambda$ is expected to lead to an increased population at the target site. Finally, it is expected that for the dephasing rate $\gamma \gg \Lambda$ diminished population arrives at the target site, since quantum transport is suppressed by the Zeno effect.

FIG. 3. Sketch of the basic processes in excitonic energy transfer. Confer to Table 1 in the main text (or Table S1) for numerical values of the time scales of the respective processes. Let $|g\rangle$ be the electronic ground state and $|M\rangle$ and $|N\rangle$ be two delocalized electronic excited states. (a) Decay between an excited state and the ground state, characterized with the decay time $T_1$ (Another name for this process is exciton recombination). (b) Dephasing of a superposition between ground state and an excited state. This process usually happens on a very fast time scale and is not relevant for the present discussion. (c) Decay in the single exciton manifold without the loss of the excitation to the ground state, characterized by the decay time between exciton states. (d) Dephasing in the single exciton manifold. Consider a superposition of exciton states $|\psi\rangle = \frac{1}{\sqrt{2}} (|M\rangle + |N\rangle)$. Then this dephasing process causes the initial density matrix $|\psi\rangle\langle\psi|$ to decay to an equal mixture $1/2(|M\rangle\langle M| + |N\rangle\langle N|)$ at long times. The time scale of this process is characterized by the dephasing time in the single exciton manifold.


<table>
<thead>
<tr>
<th>Parameter</th>
<th>FMO model</th>
<th>Quantum simulator</th>
</tr>
</thead>
<tbody>
<tr>
<td>decay time ((T_1)) ((\text{single site electron-hole recombination}))</td>
<td>(\approx\ ns)</td>
<td>(\approx 10\ \mu s)</td>
</tr>
<tr>
<td>average exciton transfer time ((\text{from site 8 to site 3}))</td>
<td>(\approx 5\ \text{ps})</td>
<td>(\approx 25\ \text{ns})</td>
</tr>
<tr>
<td>decay time between the exciton states ((\text{jump between exciton states}))</td>
<td>(\approx\ \text{ps})</td>
<td>(\approx 5\ \text{ns})</td>
</tr>
<tr>
<td>dephasing in exciton manifold ((\text{pure dephasing}))</td>
<td>(\approx 100\ \text{fs})</td>
<td>(\approx 500\ \text{ps})</td>
</tr>
<tr>
<td>time scale of quantum beatings ((\tau_{osc}))</td>
<td>(\approx 200\ \text{fs})</td>
<td>(\approx 1\ \text{ns})</td>
</tr>
<tr>
<td>coupling between sites</td>
<td>(\approx 10\ \text{cm}^{-1} - 122\ \text{cm}^{-1})</td>
<td>(\approx 60\ \text{MHz} - 730\ \text{MHz})</td>
</tr>
<tr>
<td>relative static site energy shifts</td>
<td>(\approx 10\ \text{cm}^{-1} - 500\ \text{cm}^{-1})</td>
<td>(\approx 60\ \text{MHz} - 3\ \text{GHz})</td>
</tr>
<tr>
<td>(</td>
<td>\bar{\epsilon}_i - \bar{\epsilon}_j</td>
<td>\equiv</td>
</tr>
<tr>
<td>dynamic fast fluctuations ([6]) ((\text{dephasing rate}))</td>
<td>(\approx 208\ \text{cm}^{-1}) (60\ \text{mk} \approx 1.2\ \text{GHz})</td>
<td>(100\ \text{K} \approx 69.5\ \text{cm}^{-1}) (20\ \text{mk} \approx 417\ \text{MHz})</td>
</tr>
<tr>
<td>temperature</td>
<td>(77\ \text{K} \approx 53\ \text{cm}^{-1}) (15\ \text{mk} \approx 317\ \text{MHz})</td>
<td></td>
</tr>
</tbody>
</table>

TABLE I. Comparison of parameters for the FMO complex and the quantum simulator. The timescales shown below are for the dressed states of flux qubits coupled to the quantum harmonic oscillators. Notice that the decay time in a single qubit \((T_1)\) does not need to be mapped directly from the FMO dynamics. With nowadays achievable decay times in superconducting qubits, which are 3 orders of magnitude larger than the excitation transfer time between the qubits, the dynamics of the FMO complex can be simulated.
### FMO complex

<table>
<thead>
<tr>
<th>Oscillator No.</th>
<th>Transition Frequency</th>
<th>Coupling Strength</th>
<th>Quality Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\approx 27 \text{ cm}^{-1}$</td>
<td>$\approx 2.42 \text{ cm}^{-1}$</td>
<td>$\approx 0.67$</td>
</tr>
<tr>
<td>2</td>
<td>$\approx 74 \text{ cm}^{-1}$</td>
<td>$\approx 8.60 \text{ cm}^{-1}$</td>
<td>$\approx 0.49$</td>
</tr>
<tr>
<td>3</td>
<td>$\approx 140 \text{ cm}^{-1}$</td>
<td>$\approx 11.98 \text{ cm}^{-1}$</td>
<td>$\approx 0.47$</td>
</tr>
<tr>
<td>4</td>
<td>$\approx 246 \text{ cm}^{-1}$</td>
<td>$\approx 14.10 \text{ cm}^{-1}$</td>
<td>$\approx 0.80$</td>
</tr>
<tr>
<td>5</td>
<td>$\approx 380 \text{ cm}^{-1}$</td>
<td>$\approx 10.00 \text{ cm}^{-1}$</td>
<td>$\approx 1.27$</td>
</tr>
<tr>
<td>6</td>
<td>$\approx 560 \text{ cm}^{-1}$</td>
<td>$\approx 5.40 \text{ cm}^{-1}$</td>
<td>$\approx 1.84$</td>
</tr>
</tbody>
</table>

### Quantum simulator

<table>
<thead>
<tr>
<th>Oscillator No.</th>
<th>Transition Frequency</th>
<th>Coupling Strength</th>
<th>Quality Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\approx 162 \text{ MHz}$</td>
<td>$\approx 14.50 \text{ MHz}$</td>
<td>$\approx 0.67$</td>
</tr>
<tr>
<td>2</td>
<td>$\approx 444 \text{ MHz}$</td>
<td>$\approx 51.56 \text{ MHz}$</td>
<td>$\approx 0.49$</td>
</tr>
<tr>
<td>3</td>
<td>$\approx 839 \text{ MHz}$</td>
<td>$\approx 71.83 \text{ MHz}$</td>
<td>$\approx 0.47$</td>
</tr>
<tr>
<td>4</td>
<td>$\approx 1.5 \text{ GHz}$</td>
<td>$\approx 84.54 \text{ MHz}$</td>
<td>$\approx 0.80$</td>
</tr>
<tr>
<td>5</td>
<td>$\approx 2 \text{ GHz}$</td>
<td>$\approx 59.95 \text{ MHz}$</td>
<td>$\approx 1.27$</td>
</tr>
<tr>
<td>6</td>
<td>$\approx 3 \text{ GHz}$</td>
<td>$\approx 32.38 \text{ MHz}$</td>
<td>$\approx 1.84$</td>
</tr>
</tbody>
</table>

TABLE II. Decomposition of the temperature-dependent super-Ohmic mode density at 300 K shown in Figure 4 (a) of the main article and simulation with 6 LRC-oscillators coupled to each flux qubit, see Figure 2 (a) of the main article.
### FMO complex

<table>
<thead>
<tr>
<th>Oscillator No.</th>
<th>Transition Frequency</th>
<th>Coupling Strength</th>
<th>Quality Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\approx 20 \text{ cm}^{-1}$</td>
<td>$\approx 3.0 \text{ cm}^{-1}$</td>
<td>$\approx 0.93$</td>
</tr>
<tr>
<td>2</td>
<td>$\approx 37 \text{ cm}^{-1}$</td>
<td>$\approx 5.9 \text{ cm}^{-1}$</td>
<td>$\approx 1.35$</td>
</tr>
<tr>
<td>3</td>
<td>$\approx 72 \text{ cm}^{-1}$</td>
<td>$\approx 9.7 \text{ cm}^{-1}$</td>
<td>$\approx 1.89$</td>
</tr>
<tr>
<td>4</td>
<td>$\approx 118 \text{ cm}^{-1}$</td>
<td>$\approx 7.8 \text{ cm}^{-1}$</td>
<td>$\approx 4.00$</td>
</tr>
<tr>
<td>5</td>
<td>$\approx 142 \text{ cm}^{-1}$</td>
<td>$\approx 2.8 \text{ cm}^{-1}$</td>
<td>$\approx 9.00$</td>
</tr>
<tr>
<td>6</td>
<td>$\approx 190 \text{ cm}^{-1}$</td>
<td>$\approx 16.5 \text{ cm}^{-1}$</td>
<td>$\approx 5.00$</td>
</tr>
<tr>
<td>7</td>
<td>$\approx 237 \text{ cm}^{-1}$</td>
<td>$\approx 10.4 \text{ cm}^{-1}$</td>
<td>$\approx 8.80$</td>
</tr>
<tr>
<td>8</td>
<td>$\approx 260 \text{ cm}^{-1}$</td>
<td>$\approx 6.1 \text{ cm}^{-1}$</td>
<td>$\approx 10.80$</td>
</tr>
<tr>
<td>9</td>
<td>$\approx 282 \text{ cm}^{-1}$</td>
<td>$\approx 9.9 \text{ cm}^{-1}$</td>
<td>$\approx 11.75$</td>
</tr>
<tr>
<td>10</td>
<td>$\approx 325 \text{ cm}^{-1}$</td>
<td>$\approx 4.8 \text{ cm}^{-1}$</td>
<td>$\approx 18.06$</td>
</tr>
<tr>
<td>11</td>
<td>$\approx 363 \text{ cm}^{-1}$</td>
<td>$\approx 6.3 \text{ cm}^{-1}$</td>
<td>$\approx 20.17$</td>
</tr>
<tr>
<td>12</td>
<td>$\approx 380 \text{ cm}^{-1}$</td>
<td>$\approx 5.3 \text{ cm}^{-1}$</td>
<td>$\approx 29.23$</td>
</tr>
<tr>
<td>13</td>
<td>$\approx 426 \text{ cm}^{-1}$</td>
<td>$\approx 4.4 \text{ cm}^{-1}$</td>
<td>$\approx 30.43$</td>
</tr>
<tr>
<td>14</td>
<td>$\approx 478 \text{ cm}^{-1}$</td>
<td>$\approx 3.4 \text{ cm}^{-1}$</td>
<td>$\approx 48.00$</td>
</tr>
<tr>
<td>15</td>
<td>$\approx 500 \text{ cm}^{-1}$</td>
<td>$\approx 1.3 \text{ cm}^{-1}$</td>
<td>$\approx 35.71$</td>
</tr>
</tbody>
</table>

### Quantum simulator

<table>
<thead>
<tr>
<th>Oscillator No.</th>
<th>Transition Frequency</th>
<th>Coupling Strength</th>
<th>Quality Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\approx 120 \text{ MHz}$</td>
<td>$\approx 18.00 \text{ MHz}$</td>
<td>$\approx 0.93$</td>
</tr>
<tr>
<td>2</td>
<td>$\approx 222 \text{ MHz}$</td>
<td>$\approx 35.38 \text{ MHz}$</td>
<td>$\approx 1.35$</td>
</tr>
<tr>
<td>3</td>
<td>$\approx 432 \text{ MHz}$</td>
<td>$\approx 58.16 \text{ MHz}$</td>
<td>$\approx 1.89$</td>
</tr>
<tr>
<td>4</td>
<td>$\approx 707 \text{ MHz}$</td>
<td>$\approx 46.77 \text{ MHz}$</td>
<td>$\approx 4.00$</td>
</tr>
<tr>
<td>5</td>
<td>$\approx 851 \text{ MHz}$</td>
<td>$\approx 16.79 \text{ MHz}$</td>
<td>$\approx 9.00$</td>
</tr>
<tr>
<td>6</td>
<td>$\approx 1.1 \text{ GHz}$</td>
<td>$\approx 98.93 \text{ MHz}$</td>
<td>$\approx 5.00$</td>
</tr>
<tr>
<td>7</td>
<td>$\approx 1.4 \text{ GHz}$</td>
<td>$\approx 62.36 \text{ MHz}$</td>
<td>$\approx 8.80$</td>
</tr>
<tr>
<td>8</td>
<td>$\approx 1.6 \text{ GHz}$</td>
<td>$\approx 36.57 \text{ MHz}$</td>
<td>$\approx 10.80$</td>
</tr>
<tr>
<td>9</td>
<td>$\approx 1.7 \text{ GHz}$</td>
<td>$\approx 59.36 \text{ MHz}$</td>
<td>$\approx 11.75$</td>
</tr>
<tr>
<td>10</td>
<td>$\approx 1.9 \text{ GHz}$</td>
<td>$\approx 28.78 \text{ MHz}$</td>
<td>$\approx 18.06$</td>
</tr>
<tr>
<td>11</td>
<td>$\approx 2.2 \text{ GHz}$</td>
<td>$\approx 37.77 \text{ MHz}$</td>
<td>$\approx 20.17$</td>
</tr>
<tr>
<td>12</td>
<td>$\approx 2.3 \text{ GHz}$</td>
<td>$\approx 31.79 \text{ MHz}$</td>
<td>$\approx 29.23$</td>
</tr>
<tr>
<td>13</td>
<td>$\approx 2.6 \text{ GHz}$</td>
<td>$\approx 26.38 \text{ MHz}$</td>
<td>$\approx 30.43$</td>
</tr>
<tr>
<td>14</td>
<td>$\approx 2.9 \text{ GHz}$</td>
<td>$\approx 20.39 \text{ MHz}$</td>
<td>$\approx 48.00$</td>
</tr>
<tr>
<td>15</td>
<td>$\approx 3 \text{ GHz}$</td>
<td>$\approx 7.79 \text{ MHz}$</td>
<td>$\approx 35.71$</td>
</tr>
</tbody>
</table>

**TABLE III.** Decomposition of the temperature-dependent experimental [2] mode density at 300 K shown in Figure 4 (b) of the main article and simulation with 15 LRC-oscillators coupled to each flux qubit, see Figure 2 (a) of the main article.