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Quantum biology: explore quantum dynamics in biological systems

Jianming CAI[1,2]

[1]*School of Physics, Huazhong University of Science and Technology, Wuhan* 430074*, China;*
[2]*Center of Quantum Optics Science, Huazhong University of Science and Technology, Wuhan* 430074*, China*

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Abstract In recent years, people have been extending the concepts developed in quantum information science to explore quantum dynamics in biological systems. The existence of quantum coherence in certain biological processes has been identified in a number of experiments. The role of quantum coherence and quantum entanglement has been carefully investigated, which suggests that quantum effect is important in these processes although in a more complicated way. In the mean time, these findings urge the development of new experiment methodology to reveal more biological scenarios in which quantum effect exists and plays a non-trivial role. In this article, we review the latest progress in the field of quantum biology and discuss the key challenges in further development of quantum biology.

Keywords quantum information, quantum biology, quantum optics, quantum coherence, quantum physics

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1 Introduction

Quantum biology is a recently emerging research field that mainly aims to explore the non-trivial role of quantum effect in biological systems [1–5]. The US Defense Advanced Research Program Agency (DARPA) initiated the QuBE program (Quantum Effects in Biological Environment) in 2010. On one hand, it is not very surprising that quantum mechanics is essential in biology and chemistry. For example, the nature of chemical bonding and also every chemical process involve the principles of quantum mechanics. People have been developing various techniques to study these principles in the field of quantum chemistry, and have achieved great success for those relatively large molecules. On the other hand, quantum mechanics is actually not necessary in most scenarios of biology, for example, on the level of proteins and cells. It seems that almost all processes can and will be well understood in classical biology, in particular on the physiological level. Nevertheless, there are a few pieces of evidence, including quantum energy transport in photosynthesis, magnetic sensing in birds, and phonon-assisted tunneling in olfaction, which suggest that quantum effect may have to be taken into account even in proteins and cells. Such a fact may remind us the small clouds of blackbody radiation and photoelectric effect over

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Email: jianmingcai@hust.edu.cn

the blue sky of classical mechanics in the last quarter of the nineteenth century, which in the end led to the birth of quantum mechanics.

The first key issue in the field of quantum biology thus is about the length scale where to explore quantum effect. In fact, quantum chemistry software, which incorporates quantum features, works very well for small molecules, typical on the order of less than 1nm, with a small number of atoms. However, quantum chemistry technique would require an exceptional amount of computational power when considering a typical protein (5–10 nm). Usually, a hybrid method of classical and quantum calculation is exploited. Namely a small region is calculated quantum mechanically, while the much larger surrounding system is calculated classically. This obviously raises the question: whether quantum effect that is neglected in such simulations would affect the correctness of the predictions of these systems? The hybrid method of classical and quantum calculation does result in great success in e.g., supra-molecular chemistry. Nevertheless, it remains unclear whether the treatment will be precise when applying to complex proteins. Recently, the experiment evidence suggests that quantum dynamics are crucial to the function of certain proteins and may be optimized to achieve the best efficiency [3–5]. The question whether quantum effect may exist and play a role in protein function is related to another fundamental problem in quantum mechanics: where is the border between the quantum and classical world [6]. When we increase the system size until a certain length scale, classical mechanics would become sufficient to describe the system's behavior, otherwise we need quantum mechanics in order to make correct predictions for the system. But it is unclear what is the critical length scale at the border between the quantum and the classical world. Biological systems such as proteins seem to be the right systems where the quantum world may meet the classical world.

The second key issue in the field of quantum biology is whether and how quantum effect can sustain in biological systems. Biological systems are open systems as supplied with energy. Moreover, biological systems are warm, namely at room temperature, wet and noisy with a huge number of collision events happening, which means that they are subject to a significant high level of environment fluctuations. Quantum features, such as quantum coherence and quantum correlation, however, were thought to be and indeed very fragile to thermal fluctuations and other source of noise. For example, many experiments particularly in quantum information processing allowing the observation of quantum phenomenon usually are performed in carefully isolated setups and operating at low temperature to protect systems from the environment noise so that quantum effect can be preserved for a sufficient long time. Thus, at first sight, it seems that quantum coherence and quantum entanglement is unlikely if not possible to sustain in biological systems. Nevertheless, there are evidences suggesting that proteins may mitigate and also make use of environment noise to harness quantum effect for the improvement and optimum of biological efficiency. One essential point here is quantum effect shall be relevant as long as the time scale quantum effect persistence is comparable with the time scale over which the protein function happens, even the absolute coherence time may be short. This is similar as the scenario in quantum information processing, where the coherence time is long enough as long as it is sufficient to implement for the desired quantum operations.

In this review, we present the recent advance in three representative examples, including quantum energy transport in photosynthesis (Section 2), magnetic sensing in birds (Section 3) and phonon-assisted tunneling in olfaction (Section 4). We also discuss the challenges and opportunities in the field of quantum biology (Section 5).

2 Quantum energy transport in photosynthesis

The photosynthetic machinery in plants provides almost the entire energy available to all life on the Earth's surface by harvesting sunlight. The energy from sunlight is absorbed in a chlorophyll molecule, which leads to the creation of an excited electron ("exciton") [7]. The exciton energy is transported in the system of connected chlorophylls in a very efficient way to a reaction center where the energy is used to induce charge separation [8], see Figure 1. Remarkably, the efficiency of such energy transfer is

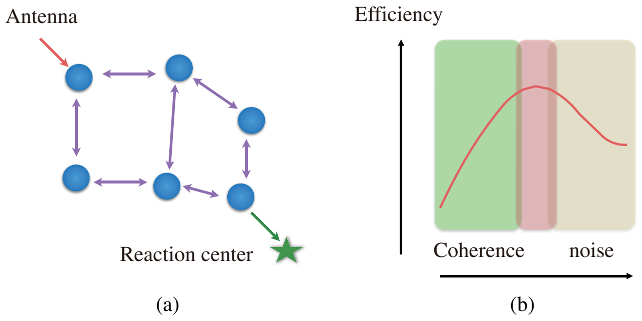

Figure 1 (Color online) (a) The schematic picture of the Bchla arrangement in the Fenna-Matthews-Olson complex. The specific electronic structure of the FMO complex determines that the excitations arrive at the one of the Bchla molecules, and transfers through the connected Bchla molecule network to the reaction center where a charge separation process starts. (b) shows the efficiency of energy transfer through the FMO complex versus the strength of noise due to the interaction between the electronic states and the protein environment. Perfect quantum coherence (i.e., no noise) or very strong noise is not beneficial for the efficient energy transfer. The interplay between quantum coherence and environment noise results in the optimal operating regime. Figure produced from [13, 14].

near 100%, namely almost every absorbed photon will be transferred to the reaction center, albeit the electronic excitation will lose energy very fast during the transfer process (on the time scale of 1 ns). This indicates that the exciton energy somehow finds an extremely efficient way to transport to the reaction center. Indeed, the experiments demonstrated that the energy transport time scale is on the order of ps [9].

A natural question thus arises, namely how can the energy transport in the connected chlorophylls network so efficient? In 2007, G. Fleming and coworkers demonstrated experimentally that quantum coherence persists in the energy transfer in the Fenna-Matthews-Olson (FMO) complex over the time scale also on the order of ps [9]. The exciton actually delocalizes over several chlorophylls instead of on a single chlorophyll. They also hinted that the excitation might explore different transport paths simultaneously in a coherent way, so as to achieve the very high efficiency of energy transfer. Since this breakthrough, more experiments have demonstrated quantum coherence in other photosynthetic systems even at room temperature [10–12].

The two main problems in the context of quantum energy transport in photosynthetic systems are (1) what enables quantum coherence to sustain in photosynthetic systems? (2) whether and how quantum coherence helps to achieve highly efficient quantum energy transport in photosynthetic systems? A lot of literatures have targeted to answer these two problems [13–29]. All these studies have revealed an intriguing fact that it is quite likely that protein environment is the key element to provide the answers. The Hamiltonian that describes the exciton-exciton interaction is written as follows [18]

$$H_s = \sum_{j=1}^{N} E_j |j\rangle\langle j| + \sum_{j\neq k} g_{jk}(|j\rangle\langle k| + |k\rangle.\langle j|). \tag{1}$$

People find that the above coherent part of the system dynamics is not enough to explain the high efficiency of energy transfer. It was suggested that the non-Markovian and non-perturbative protein environment plays an important role in the survival of quantum coherence and in the enhancement of energy transfer efficiency [16, 17]. Most recently, a new analysis suggested that if the protein vibrational mode energy matches the electronic energy difference in different chromophores, a long-lived vibration would drive coherent oscillation between electronic excitations in a light-harvesting complex [27–29]. It is such interplay between the electronic excitation and the protein vibration mode that leads to the survival of quantum coherence at room temperature in these photosynthetic systems.

Although the conclusive answers to the above two key questions are not clear, it already demonstrates that the role of quantum coherence in photosynthetic systems is remarkably different from its role in quantum information processing. In that context, much effort has been invested to preserve quantum coherence and quantum entanglement for long periods so that one may implement as many quantum

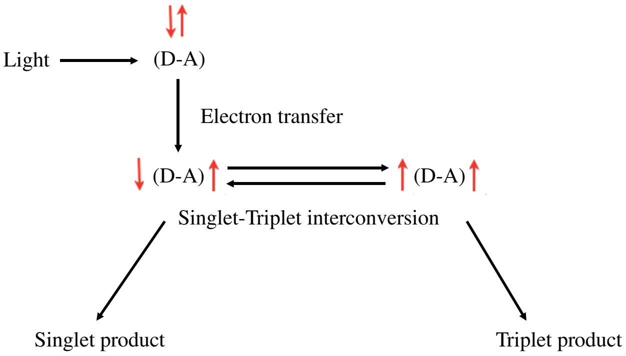

Figure 2 (Color online) The operating principle of the radical pair mechanism for magnetoreception in birds. Light induced electron transfer from a donor (D) to an acceptor (A) molecule creates a radical pair, usually in the singlet state. The evolution of the radical pair spin state is governed by both the external magnetic field and the interaction with the surrounding nuclear environment. Figure produced from [33].

operations as possible. In contrast, environment noise is not simply bad in quantum energy transport in photosynthesis. It appears that nature has managed to tune the protein environment to match the electronic structure or vice versa. In this way, quantum coherence is maintained to the most suitable extension and is harnessed to optimize the energy transfer efficiency.

3 Magnetic sensing in birds

People have found that many migrating species use a magnetic compass to help them create a magic map using the Earth's magnetic field. The precise molecular mechanism underlying such (bio)magnetoreception, however, remains unclear. Behavior experiments suggest that birds quite likely use several mechanisms to acquire the direction information. The most attractive and favorite mechanism is the radical pair mechanics involving electron spins [30–38].

The operating principle of the radical pair mechanism, see Figure 2, is as follows [39,40]: a photochemical reaction starts from the light activation of a photoreceptor, and is followed by an electron transfer process; a radical pair then carries two unpaired electrons in a spin-correlated electronic singlet state. Each radical (i.e., unpaired electron) has spin-1/2; initially the spins of the radical pair are in the singlet state, which is called maximally entangled state in quantum information science. Under the combined action of the external magnetic field (e.g., the Earth's magnetic field) and importantly also the hyperfine interaction with local nuclei in the molecule backbone, the radical pair starts to evolve from the singlet state to the triplet state, and vice versa. The system Hamiltonian is given by [39, 40]

$$H = H_0 + \hat{B}, \tag{2}$$

$$H_0 = \sum_{k=D,A} \sum_j \vec{s}_k \cdot \hat{T}_{kj} \cdot \vec{I}_{k_j}, \tag{3}$$

$$\hat{B} = -g\mu_b \vec{b} \cdot (\vec{s}_D + \vec{s}_A). \tag{4}$$

The rate of such a photochemical reaction is affected by the spin state of radical electrons. Namely, the reaction rate and/or the reaction path are dependent on whether the radical pair spins are in the singlet state or in the triplet state. Therefore, the reaction product is controlled by both the strength and the orientation of the external magnetic field with respect to the molecular frame. It was hypothesized that the radical pair reaction product is further converted to nerve signal and thus birds may obtain information on the Earth's magnetic field to guide their migration [33].

The radical pair mechanism was promoted by a number of behavior experiments. It was demonstrated that the magnetic compass in European robins acts as an inclination compass rather than a polarity compass. The functioning of such a magnetic compass was shown to be sensitive to the wavelength of light [32]. Another encouraging evidence is that experiments had shown that very weak radio-frequency

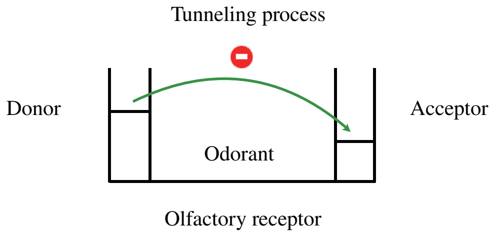

Figure 3 (Color online) The vibrational olfaction mechanism based on inelastic electron tunneling. An electron could efficiently tunnel quantum mechanically from a donor to an acceptor site within the protein if the vibration frequency of the odorant matches the energy difference between the donor and acceptor. Figure produced from [47, 48].

field would disrupt navigation if its frequency matches the Zeeman splitting between the spin-up and spin-down of radical electrons in the Earth's magnetic field [31]. Although people have not managed to identify the right candidate molecule for the radical pair mechanism, Maeda et al. [41] reported a triad molecule composed of linked carotenoid (C), porphyrin (P) and fullerene (F) which showed a magnetic field sensitivity down to 50 μT (similar to the geomagnetic field) .

In the radical pair mechanism, the radical pair spin state shows the character of singlet or triplet state that is maximally entangled in quantum information science. As decoherence will diminish the coherent inter-conversion between the singlet and triplet state, it will prevent the radical pair reaction from being susceptive to very weak radio frequency disrupting fields. Based on the experimental evidence that the disrupting radio frequency fields were as weak as 50–100 nT [31], it was argued that quantum coherence of radical pair spins has to sustain for tens of microseconds so that the disrupting radio frequency fields have enough time to take effect [42, 43]. This is a quite amazing result for electron spin in warm and noisy biological environment as coherence times on the order of tens of microseconds are quite difficult to achieve for man-made electron spin systems. More work needs to be done to further support such a statement. If it was true, how nature can achieve this amazingly long spin coherence time remains a mystery. The specific features of protein environment may play an important role for the survival of radical pair spin coherence.

The second important problem is about the role of quantum coherence and/or quantum entanglement in the radical pair mechanism [44–46]. It was shown that quantum coherence itself might not be very essential for the functioning of a radical pair magnetic compass [44]. The interplay between quantum coherence and the environment noise is the key to achieve its high magnetic sensitivity. By introducing the concept of global quantum coherence, it was found that the essence of the radical pair magnetic compass model can be understood in analogy to a quantum interferometer exploiting global quantum coherence rather than any subsystem coherence, namely the more global quantum coherence the better performance a radical pair magnetic compass can achieve [46].

4 Phonon-assisted tunneling in olfaction

Olfaction (the sense of smell) is the ultimate molecular recognition system that can detect and identify thousands of molecules. There are hundreds of receptors that bind odorant molecules. It remains a mystery how such binding is translated into a sense of smell. The most familiar principle is the "lock and key" principle, namely the molecule shape determines the odour. It is the structural features of odorants that are recognized by the receptors and result in a smell character. The "lock and key" principle was, however, challenged by the observation that some odorants with the hydrogens replaced with the heavier isotope deuterium, which leaves its shape unchanged, but smells very different. This fact cannot be explained by the "lock and key" principle. The other mechanism suggested that the receptors bind the odorants, then an electron tunnel quantum mechanically from a donor to an acceptor site, see Figure 3, which is affected by the molecular vibrations [47, 48]. The rate of electron tunneling across the odorant from a donor to an acceptor site within the protein depends on whether the energy difference between the donor and acceptor can be compensated by a vibration energy of the odorant. This vibrational olfaction mechanism can explain, when the hydrogens in acetophenone are replaced with the heavier isotope deuterium, the smell becomes rather different. Recently, experiments showed that fruit flies can 'smell' molecular vibrations, which provides an evidence to support the vibrational olfaction mechanism.

5 Challenges and opportunities

Although there is intensive research going on in the field of quantum biology, particularly in the above three specific examples, the understanding of these phenomena is far from satisfactory. In the experiments, which observed quantum coherent energy transfer in photosynthetic systems, the excitations are created with laser pulses. However, in real photosynthetic systems, the excitations are generated by (incoherent) sunlight. It is not clear how quantum coherence is preserved and whether it still plays a significant role in this scenario. In the magnetoreception of birds, the experiments that demonstrated weak resonant radio frequency fields disrupt navigation were regarded as direct and strong evidence for a radical pair magnetic sensing mechanism. However, more recent work showed that weak radio frequency noise and/or electric noise at most frequencies can be as disruptive as the resonant weak radio frequency disruptive field. How does this result reconcile with the previous experiment, and how is it consistent with the radical pair mechanics is not clear. People have realized that the complex protein environment shall play a significant role. It remains a challenging task to accurately model such a complex environment and to incorporate into the relevant quantum dynamics.

The more challenging tasks are on the experimental side. One would like to collect more direct evidences for the existence and the role of quantum effect in real biological processes. It is also important to get more information about the relevant protein environment directly in experiment. However, the measurement methods and techniques that people have developed for the observation of quantum dynamics in well-isolated systems may not be easily extended to mesoscopic and complex biological systems at ambient condition. The measurement and control methods that are applicable to the investigation of quantum dynamics in biologically shall work at room temperature and at nanometer scale, namely (single molecule) nano-measurement. One of the candidate techniques is an individually addressable spin sensor as exemplified by nitrogen vacancy in nanodiamonds that satisfy these two requirements. More powerful techniques need to be devised and developed in experiments. Furthermore, it is equally important to find ways to probe and control not only the systems but also the (protein) environment, which significantly affect the functioning of quantum bioprocesses.

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