

Kuantum Kaynak Teorilerine Giriş

KUANTUM BİYOLOJİ

⟨ QSB | KU ⟩

Dr. Onur Pusuluk

Koç Üniversitesi

11 Nisan 2021



Prolog

1. Kuantum Devriminde Biyoloji

Monolog

2. Kuantum Devriminde Biyoloji

Diyaloglar

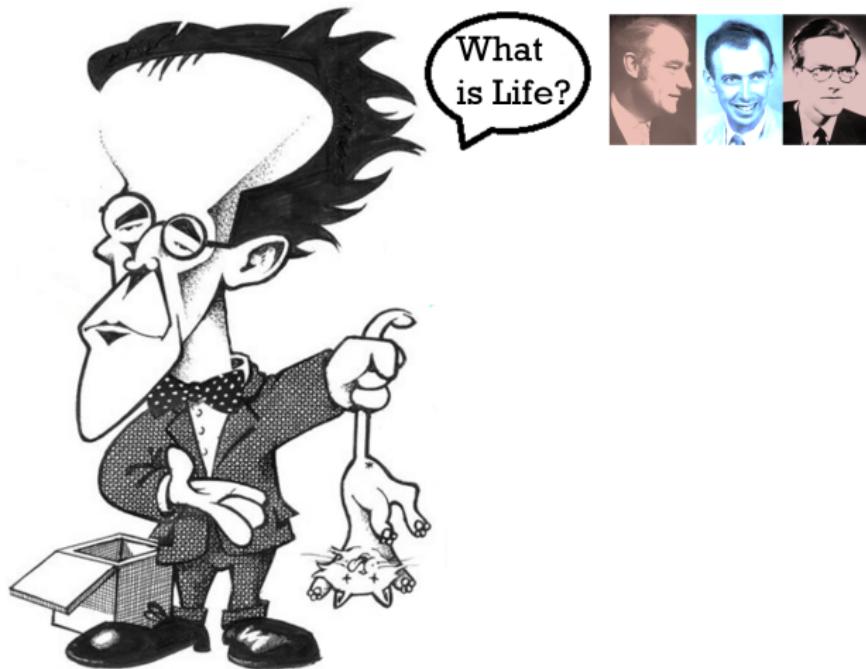
“Kuantum” Manyetik Duyum

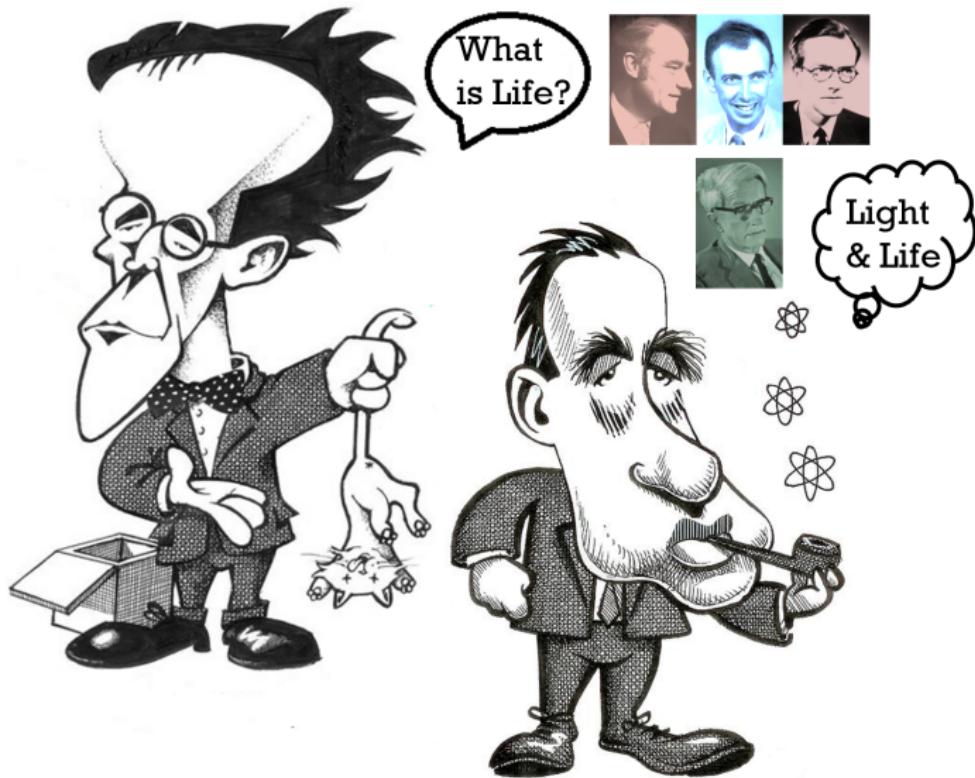
“Kuantum” Görme

“Kuantum” Koku Alma

Epilog

Kuantum Hesapsal Kimya







The Nobel Prize in Chemistry 1954

Linus Pauling

Share this:      33

The Nobel Prize in Chemistry 1954



Linus Carl Pauling

Prize share: 1/1

The Nobel Prize in Chemistry 1954 was awarded to Linus Pauling "for his research into the nature of the chemical bond and its application to the elucidation of the structure of complex substances".

Photos: Copyright © The Nobel Foundation



The Nobel Prize in Chemistry 1954

Linus Pauling

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The Nobel Prize in Chemistry 1954



Linus Carl Pauling

Prize share: 1/1

The Nobel Prize in Chemistry 1954 was awarded to Linus Pauling "for his research into the nature of the chemical bond and its application to the elucidation of the structure of complex substances".

Photos: Copyright © The Nobel Foundation



kimyasal bağ

- ▶ hibritleşme
- ▶ elektronegatiflik
- ▶ rezonans



The Nobel Prize in Chemistry 1954
Linus Pauling

Share this: 33

The Nobel Prize in Chemistry 1954



Linus Carl Pauling
Prize share: 1/1

The Nobel Prize in Chemistry 1954 was awarded to Linus Pauling "for his research into the nature of the chemical bond and its application to the elucidation of the structure of complex substances".

Photos: Copyright © The Nobel Foundation

"It is convenient to consider three extreme types of chemical bonds: electrostatic bonds, covalent bonds, and metallic bonds. This classification is not rigorous one; for, although the bonds of each extreme type have well-defined properties, the transition from one extreme type to another may be gradual, permitting the existence of bonds of intermediate type."



The Nobel Prize in Chemistry 1954
Linus Pauling

Share this: [f](#) [g+](#) [t](#) [+](#) [e](#) 33

The Nobel Prize in Chemistry 1954



Linus Carl Pauling
Prize share: 1/1

The Nobel Prize in Chemistry 1954 was awarded to Linus Pauling "for his research into the nature of the chemical bond and its application to the elucidation of the structure of complex substances".

Photos: Copyright © The Nobel Foundation



moleküler yapı

- ▶ α sarmal & β yaprak
- ▶ üçlü DNA sarmalı
- ▶ yapısal tamamlayıcılık
 - ▶ enzim tepkimeleri
 - ▶ antijen tanıma
 - ▶ DNA replikasyonu
- ▶ moleküler genetik/tıp

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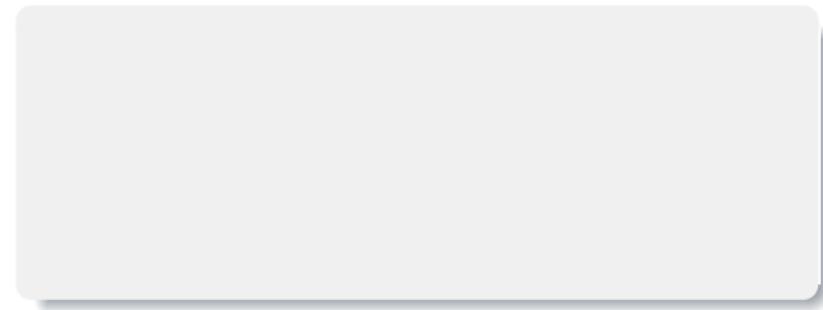
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Kuantum Hesapsal Kimya

Yöntemler & Model Süreçler



- Kuantum (Hesapsal) Kimya

- ▶ Kuantum (Hesapsal) Kimya
- ▶ (Fermiyonik) Kuantum Enformasyon

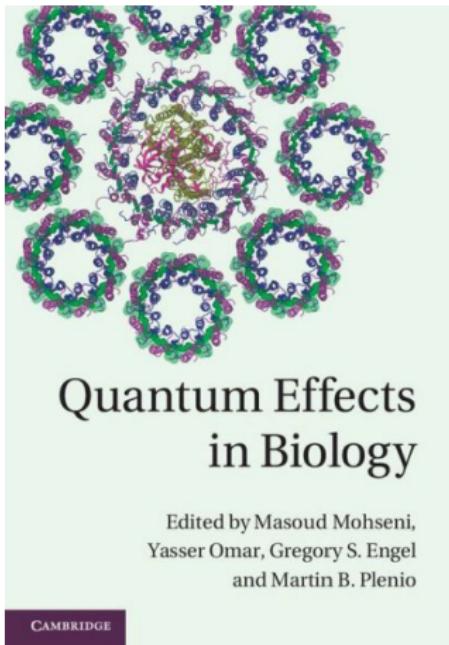
- ▶ Kuantum (Hesapsal) Kimya
- ▶ (Fermiyonik) Kuantum Enformasyon
- ▶ Açık Kuantum Sistem Dinamiği

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- ▶ (Fermiyonik) Kuantum Enformasyon
- ▶ Açık Kuantum Sistem Dinamiği
- ▶ (Single-Shot) Kuantum Termodinamik

- ▶ Kuantum (Hesapsal) Kimya
- ▶ (Fermiyonik) Kuantum Enformasyon
- ▶ Açık Kuantum Sistem Dinamiği
- ▶ (Single-Shot) Kuantum Termodinamik
- ▶ Tek Molekül Deneyleri

- ▶ Kuantum (Hesapsal) Kimya
- ▶ (Fermiyonik) Kuantum Enformasyon
- ▶ Açık Kuantum Sistem Dinamiği
- ▶ (Single-Shot) Kuantum Termodinamik
- ▶ Tek Molekül Deneyleri

- ▶ Fotosentez
- ▶ Manyetik duyum
- ▶ Görme
- ▶ Koku alma
- ▶ Biliş
- ▶ Enzim katalizi



The book cover features a light green background with several circular molecular structures composed of purple and green lines and dots. Below the image, the title 'Quantum Effects in Biology' is written in a large, bold, black serif font. At the bottom left, it says 'Edited by Masoud Mohseni, Yasser Omar, Gregory S. Engel and Martin B. Plenio' and 'CAMBRIDGE'.

**Quantum Effects
in Biology**

Edited by Masoud Mohseni,
Yasser Omar, Gregory S. Engel
and Martin B. Plenio

CAMBRIDGE

Quantum effects in biology: golden rule in enzymes, olfaction, photosynthesis and magnetodetection

Jennifer C. Brookes *Proc. R. Soc. A* **473**: 20160822.

The future of quantum biology

Adriana Marais¹, Betony Adams¹, Andrew K. Ringsmuth^{2,3,†}, Marco Ferretti², J. Michael Gruber², Ruud Hendrikx², Maria Schuld¹, Samuel L. Smith⁴, Ilya Sinayskiy^{1,5}, Tjaart P. J. Krüger⁶, Francesco Petruccione^{1,5} and Rienk van Grondelle² *J. R. Soc. Interface* **15**: 20180640.

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Modern Physics Letters B
Vol. 29 (2015) 1530013 (41 pages)
© World Scientific Publishing Company
DOI: 10.1142/S0217984915300136

Brief Review

The radical-pair mechanism as a paradigm for the emerging science of quantum biology

Iannis K. Kominis

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ikominis@physics.uoc.gr

PHYSICAL REVIEW E 80, 056115 (2009)

Quantum Zeno effect explains magnetic-sensitive radical-ion-pair reactions

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Department of Physics, University of Crete, Heraklion 71103, Greece

and Institute of Electronic Structure & Laser, Foundation for Research and Technology, Heraklion 71110, Greece

(Received 19 February 2009; revised manuscript received 13 July 2009; published 24 November 2009)

Chemical reactions involving radical-ion pairs are ubiquitous in biology, since not only are they at the basis of the photosynthetic reaction chain, but are also assumed to underlie the biochemical magnetic compass used by avian species for navigation. Recent experiments with magnetic-sensitive radical-ion-pair reactions provided strong evidence for the radical-ion-pair magnetoreception mechanism, verifying the expected magnetic sensitivities and chemical product yield changes. It is here shown that the theoretical description of radical-ion-pair reactions used since the 70s cannot explain the observed data, because it is based on phenomenological equations masking quantum coherence effects. The fundamental density-matrix equation derived here from basic quantum measurement theory considerations naturally incorporates the quantum Zeno effect and readily explains recent experimental observations on low- and high magnetic-field radical-ion-pair reactions.

DOI: [10.1103/PhysRevE.80.056115](https://doi.org/10.1103/PhysRevE.80.056115)

PACS number(s): 82.20.-w



PRL 106, 040503 (2011)

PHYSICAL REVIEW LETTERS

week ending
28 JANUARY 2011



Sustained Quantum Coherence and Entanglement in the Avian Compass

Erik M. Gauger,¹ Elisabeth Rieper,² John J. L. Morton,^{1,3} Simon C. Benjamin,^{2,1,*} and Vlatko Vedral^{2,3,4}

¹*Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom*

²*Centre for Quantum Technologies, National University of Singapore, Singapore*

³*Clarendon Laboratory, University of Oxford, Parks Road, OX1 3PU, United Kingdom*

⁴*Department of Physics, National University of Singapore, Singapore*

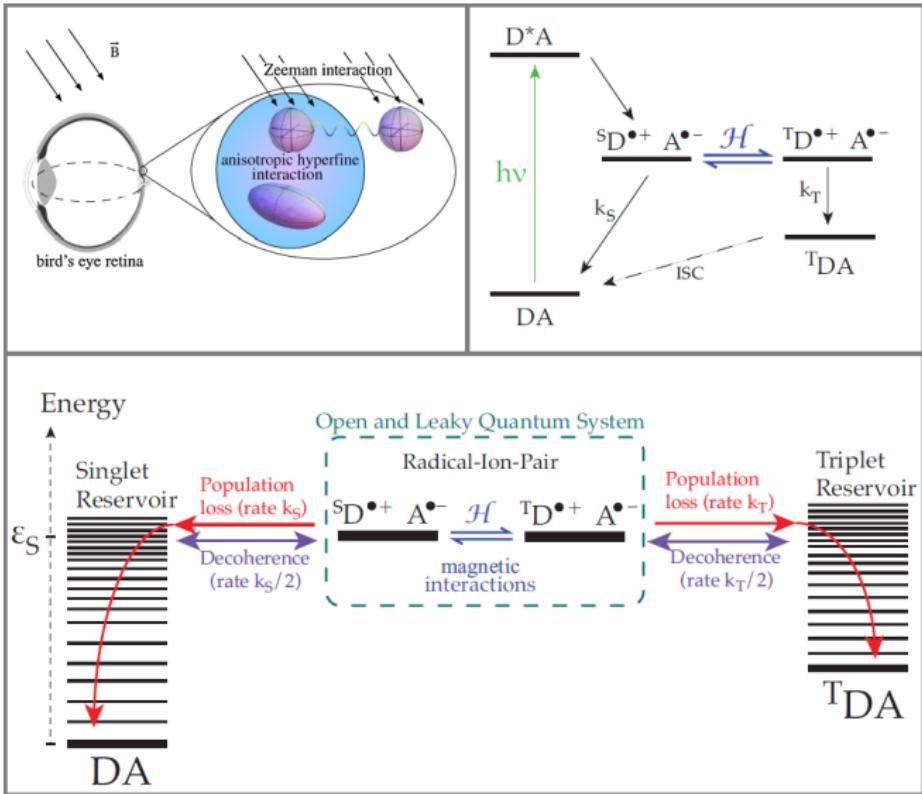
(Received 24 May 2010; revised manuscript received 23 November 2010; published 25 January 2011)

In artificial systems, quantum superposition and entanglement typically decay rapidly unless cryogenic temperatures are used. Could life have evolved to exploit such delicate phenomena? Certain migratory birds have the ability to sense very subtle variations in Earth's magnetic field. Here we apply quantum information theory and the widely accepted "radical pair" model to analyze recent experimental observations of the avian compass. We find that superposition and entanglement are sustained in this living system for at least tens of microseconds, exceeding the durations achieved in the best comparable man-made molecular systems. This conclusion is starkly at variance with the view that life is too "warm and wet" for such quantum phenomena to endure.

DOI: 10.1103/PhysRevLett.106.040503

PACS numbers: 03.67.-a, 03.65.Yz, 82.30.-b

Kuş Navigasyonu



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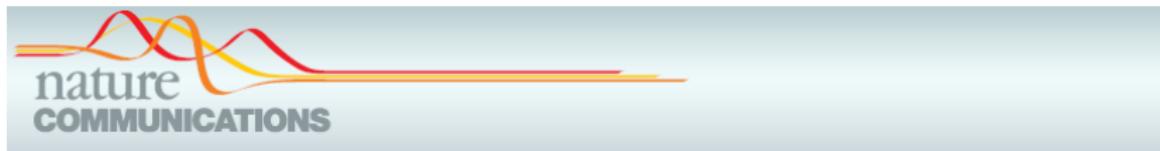
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Epilog

Kuantum Hesapsal Kimya



ARTICLE

Received 15 Jan 2016 | Accepted 7 Jun 2016 | Published 19 Jul 2016

DOI: 10.1038/ncomms12172

OPEN

Direct detection of a single photon by humans

Jonathan N. Tinsley^{1,2,†,*}, Maxim I. Molodtsov^{1,2,3,*}, Robert Prevedel^{1,2,3}, David Wartmann^{1,†}, Jofre Espigulé-Pons^{2,4}, Mattias Lauwers¹ & Alipasha Vaziri^{1,2,3,5}

NATURE COMMUNICATIONS | 7:12172 | DOI: 10.1038/ncomms12172 | www.nature.com/naturecommunications

PHYSICAL REVIEW APPLIED 8, 044012 (2017)



Quantum Biometrics with Retinal Photon Counting

M. Loulakis,^{1,*} G. Blatsios,² C. S. Vretou,³ and I. K. Kominis^{4,†}

It is known that the eye's scotopic photodetectors, rhodopsin molecules, and their associated phototransduction mechanism leading to light perception, are efficient single-photon counters. We here use the photon-counting principles of human rod vision to propose a secure quantum biometric identification based on the quantum-statistical properties of retinal photon detection. The photon path along the human eye until its detection by rod cells is modeled as a filter having a specific transmission coefficient. Precisely determining its value from the photodetection statistics registered by the conscious observer is a quantum parameter estimation problem that leads to a quantum secure identification method. The probabilities for false-positive and false-negative identification of this biometric technique can readily approach 10^{-10} and 10^{-4} , respectively. The security of the biometric method can be further quantified by the physics of quantum measurements. An impostor must be able to perform quantum thermometry and quantum magnetometry with energy resolution better than $10^{-9}\hbar$, in order to foil the device by noninvasively monitoring the biometric activity of a user.

DOI: [10.1103/PhysRevApplied.8.044012](https://doi.org/10.1103/PhysRevApplied.8.044012)

Biophysics

SEARCHING FOR PRINCIPLES

.....
William Bialek

PHYSICAL REVIEW A 101, 042116 (2020)

Editors' Suggestion

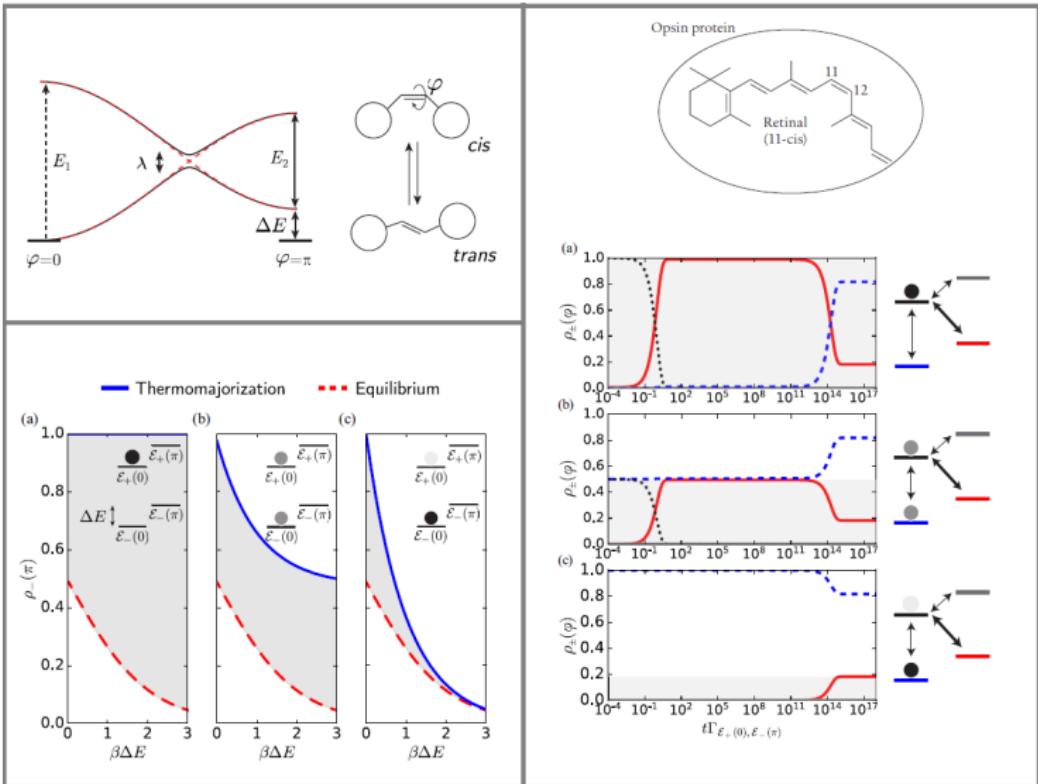
Fundamental limitations on photoisomerization from thermodynamic resource theories

Nicole Yunger Halpern^{①,2,3,4,5,*} and David T. Limmer^{⑥,7,8,†}

Small, out-of-equilibrium, and quantum systems defy simple thermodynamic expressions. Such systems are exemplified by molecular switches, which exchange heat with a bath. These molecules can photoisomerize, or change conformation, or switch, on absorbing light. The photoisomerization probability depends on kinetic details that couple the molecule's energetics to its dissipation. Therefore, a simple, general, thermodynamic-style bound on the photoisomerization probability seems out of reach. We derive such a bound using a resource theory. The resource-theory framework is a set of mathematical tools, developed in quantum information theory, used to generalize thermodynamics to small and quantum settings. From this toolkit has been derived a generalization of the second law, the thermomajorization preorder. We use thermomajorization to upper-bound the photoisomerization probability. Then, we compare the bound with an equilibrium prediction and with a Lindbladian model. We identify a realistic parameter regime in which the Lindbladian evolution saturates the thermomajorization bound. We also quantify the energy coherence in the electronic degree of freedom, and we argue that this coherence cannot promote photoisomerization. This work illustrates how quantum-information-theoretic thermodynamics can elucidate complex quantum processes in nature, experiments, and synthetics.

DOI: [10.1103/PhysRevA.101.042116](https://doi.org/10.1103/PhysRevA.101.042116)

Foto-izomerizasyon



arXiv:2103.14534v2 [quant-ph]

Non-Markovianity boosts the efficiency of bio-molecular switches

Giovanni Spaventa,* Susana F. Huelga,[†] and Martin B. Plenio[‡]

*Institute of Theoretical Physics and IQST, Universität Ulm,
Albert-Einstein-Allee 11 D-89081, Ulm, Germany*

(Dated: April 9, 2021)

Quantum resource theory formulations of thermodynamics offer a versatile tool for the study of fundamental limitations to the efficiency of physical processes, independently of the microscopic details governing their dynamics. Despite the ubiquitous presence of non-Markovian dynamics in open quantum systems at the nanoscale, rigorous proofs of their beneficial effects on the efficiency of quantum dynamical processes at the bio-molecular level have not been reported yet. Here we combine the resource theory of athermality with concepts from the theory of divisibility classes for quantum channels, to prove that memory effects can increase the efficiency of photoisomerization to levels that are not achievable under a purely Markovian (i.e. memoryless) evolution. This provides rigorous evidence that memory effects can be a useful resource in biological quantum dynamics, and, more generally, quantum thermodynamics at the nanoscale.

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Epilog

Kuantum Hesapsal Kimya

Status of the Vibrational Theory of Olfaction

Ross D. Hoehn^{1*}, David E. Nichols², Hartmut Neven³ and Sabre Kais^{1,4*}

¹ Departments of Chemistry and Physics, Purdue University, West Lafayette, IN, United States, ² Department of Pharmacology, University of North Carolina, Chapel Hill, Chapel Hill, NC, United States, ³ Google Los Angeles, Venice, CA, United States, ⁴ Santa Fe Institute, Santa Fe, NM, United States

The vibrational theory of olfaction is an attempt to describe a possible mechanism for olfaction which is explanatory and provides researchers with a set of principles which permit predictions allowing for structure-odor relations. Similar theories have occurred several times throughout olfactory science; this theory has again recently come to prominence by Luca Turin, who suggested that inelastic electron tunneling is the method by which vibrations are detected by the olfactory receptors within the nose. This work is intended to convey to the reader an up-to-date account of the vibrational theory of olfaction, both the historical iterations as well as the present iteration. This text is designed to give a chronological account of both theoretical and experimental studies on the topic, while providing context, comments, and background where they were found to be needed.

OPEN ACCESS

Edited by:

Alkwin Slenczka,
University of Regensburg, Germany

Keywords: olfaction, biophysics, vibration detection, review literature as topic, GPCRs



PRL **98**, 038101 (2007)

PHYSICAL REVIEW LETTERS

week ending
19 JANUARY 2007



Could Humans Recognize Odor by Phonon Assisted Tunneling?

Jennifer C. Brookes,^{*} Filio Hartoutsiou,[†] A. P. Horsfield,[‡] and A. M. Stoneham[§]

Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, United Kingdom

(Received 10 July 2006; published 16 January 2007)

Our sense of smell relies on sensitive, selective atomic-scale processes that occur when a scent molecule meets specific receptors in the nose. The physical mechanisms of detection are unclear: odorant shape and size are important, but experiment shows them insufficient. One novel proposal suggests receptors are actuated by inelastic electron tunneling from a donor to an acceptor mediated by the odorant, and provides critical discrimination. We test the physical viability of this mechanism using a simple but general model. With parameter values appropriate for biomolecular systems, we find the proposal consistent both with the underlying physics and with observed features of smell. This mechanism suggests a distinct paradigm for selective molecular interactions at receptors (the swipe card model): recognition and actuation involve size and shape, but also exploit other processes.

DOI: [10.1103/PhysRevLett.98.038101](https://doi.org/10.1103/PhysRevLett.98.038101)

PACS numbers: 87.16.Xa, 82.39.Jn, 87.16.Ac, 87.14.Ee

THE JOURNAL OF CHEMICAL PHYSICS 142, 025102 (2015)

Dissipation enhanced vibrational sensing in an olfactory molecular switch

Agata Chęcińska,^{1,a)} Felix A. Pollock,^{2,a)} Libby Heaney,¹ and Ahsan Nazir^{3,4}

Motivated by a proposed olfactory mechanism based on a vibrationally activated molecular switch, we study electron transport within a donor-acceptor pair that is coupled to a vibrational mode and embedded in a surrounding environment. We derive a polaron master equation with which we study the dynamics of both the electronic and vibrational degrees of freedom beyond previously employed semiclassical (Marcus-Jortner) rate analyses. We show (i) that in the absence of explicit dissipation of the vibrational mode, the semiclassical approach is generally unable to capture the dynamics predicted by our master equation due to both its assumption of one-way (exponential) electron transfer from donor to acceptor and its neglect of the spectral details of the environment; (ii) that by additionally allowing strong dissipation to act on the odorant vibrational mode, we can recover exponential electron transfer, though typically at a rate that differs from that given by the Marcus-Jortner expression; (iii) that the ability of the molecular switch to discriminate between the presence and absence of the odorant, and its sensitivity to the odorant vibrational frequency, is enhanced significantly in this strong dissipation regime, when compared to the case without mode dissipation; and (iv) that details of the environment absent from previous Marcus-Jortner analyses can also dramatically alter the sensitivity of the molecular switch, in particular, allowing its frequency resolution to be improved. Our results thus demonstrate the constructive role dissipation can play in facilitating sensitive and selective operation in molecular switch devices, as well as the inadequacy of semiclassical rate equations in analysing such behaviour over a wide range of parameters. © 2015 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4905377>]

Kokuda Moleküler Tanıma



The diagram illustrates the process of molecular detection in the nasal cavity. On the left, a profile of a human head shows a magnified view of the nasal cavity. Inside, two molecules are shown: one labeled "deuterium" with a deuterium atom (D_2) highlighted in red, and another labeled "hydrogen" with a hydrogen atom (H_2) highlighted in green. Both molecules are shown fitting into a blue puzzle piece, representing their interaction with a "protein receptor". On the right, a schematic diagram shows the nasal mucosal layer. It consists of a "Mucus layer" on top, followed by a "Lipid bilayer" containing various components: ϵ_D , ω_0 , A , M , G , T_X , T_I , T_L , T_{T0} , T_{T1} , and T_R . A wave vector v and angle X are indicated. Below this, a cross-section shows a funnel-shaped receptor site with a dipole moment δ and energy levels separated by $\frac{1}{2}\hbar\nu$.

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Tensör Ağları



JOURNAL OF CHEMICAL PHYSICS

VOLUME 110, NUMBER 9

1 MARCH 1999

Ab initio quantum chemistry using the density matrix renormalization group

Steven R. White

Department of Physics and Astronomy, University of California, Irvine, California 92697

Richard L. Martin

Theoretical Division, MSB268, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

(Received 9 November 1998; accepted 23 December 1998)

In this paper we describe how the density matrix renormalization group can be used for quantum chemical calculations for molecules, as an alternative to traditional methods, such as configuration interaction or coupled cluster approaches. As a demonstration of the potential of this approach, we present results for the H₂O molecule in a standard gaussian basis. Results for the total energy of the system compare favorably with the best traditional quantum chemical methods. © 1999 American Institute of Physics. [S0021-9606(99)31309-X]

ARTICLES

PUBLISHED ONLINE: 9 JUNE 2013 | DOI: 10.1038/NCHEM.1677

nature
chemistry

Entangled quantum electronic wavefunctions of the Mn₄CaO₅ cluster in photosystem II

Yuki Kurashige^{1*}, Garnet Kin-Lic Chan² and Takeshi Yanai¹

It is a long-standing goal to understand the reaction mechanisms of catalytic metalloenzymes at an entangled many-electron level, but this is hampered by the exponential complexity of quantum mechanics. Here, by exploiting the special structure of physical quantum states and using the density matrix renormalization group, we compute near-exact many-electron wavefunctions of the Mn₄CaO₅ cluster of photosystem II, with more than 1×10^{18} quantum degrees of freedom. This is the first treatment of photosystem II beyond the single-electron picture of density functional theory. Our calculations support recent modifications to the structure determined by X-ray crystallography. We further identify multiple low-lying energy surfaces associated with the structural distortion seen using X-ray crystallography, highlighting multistate reactivity in the chemistry of the cluster. Direct determination of Mn spin-projections from our wavefunctions suggests that current candidates that have been recently distinguished using parameterized spin models should be reassessed. Through entanglement maps, we reveal rich information contained in the wavefunctions on bonding changes in the cycle.

Sinir Ağları



RESEARCH ARTICLE

Science 355, 602–606 (2017) 10 February 2017

MANY-BODY PHYSICS

Solving the quantum many-body problem with artificial neural networks

Giuseppe Carleo^{1,*} and Matthias Troyer^{1,2}

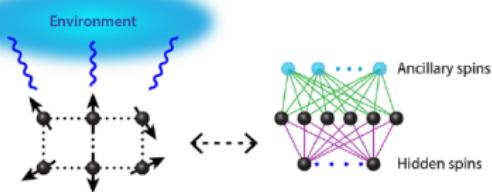
The challenge posed by the many-body problem in quantum physics originates from the difficulty of describing the nontrivial correlations encoded in the exponential complexity of the many-body wave function. Here we demonstrate that systematic machine learning of the wave function can reduce this complexity to a tractable computational form for some notable cases of physical interest. We introduce a variational representation of quantum states based on artificial neural networks with a variable number of hidden neurons. A reinforcement-learning scheme we demonstrate is capable of both finding the ground state and describing the unitary time evolution of complex interacting quantum systems. Our approach achieves high accuracy in describing prototypical interacting spins models in one and two dimensions.

VIEWPOINT

Neural Networks Take on Open Quantum Systems

Simulating a quantum system that exchanges energy with the outside world is notoriously hard, but the necessary computations might be easier with the help of neural networks.

by Maria Schuld^{*†}, Ilya Sinayskiy^{††}, and Francesco Petruccione^{¶||,**}



REFERENCES

- [3] M. J. Hartmann and G. Carleo, "Neural-network approach to dissipative quantum many-body dynamics," *Phys. Rev. Lett.* **122**, 250502 (2019).
- [4] A. Nagy and V. Savona, "Variational quantum Monte Carlo method with a neural-network ansatz for open quantum systems," *Phys. Rev. Lett.* **122**, 250501 (2019).
- [5] F. Vicentini, A. Biella, N. Regnault, and C. Ciuti, "Variational neural-network ansatz for steady states in open quantum systems," *Phys. Rev. Lett.* **122**, 250503 (2019).

NATURE COMMUNICATIONS | (2019)10:5024 | <https://doi.org/10.1038/s41467-019-12875-2> | www.nature.com/naturecommunications

Unifying machine learning and quantum chemistry with a deep neural network for molecular wavefunctions

K.T. Schütt¹, M. Gastegger¹, A. Tkatchenko^{2*}, K.-R. Müller^{1,3,4*} & R.J. Maurer^{5*}

Machine learning advances chemistry and materials science by enabling large-scale exploration of chemical space based on quantum chemical calculations. While these models supply fast and accurate predictions of atomistic chemical properties, they do not explicitly capture the electronic degrees of freedom of a molecule, which limits their applicability for reactive chemistry and chemical analysis. Here we present a deep learning framework for the prediction of the quantum mechanical wavefunction in a local basis of atomic orbitals from which all other ground-state properties can be derived. This approach retains full access to the electronic structure via the wavefunction at force-field-like efficiency and captures quantum mechanics in an analytically differentiable representation. On several examples, we demonstrate that this opens promising avenues to perform inverse design of molecular structures for targeting electronic property optimisation and a clear path towards increased synergy of machine learning and quantum chemistry.

Kuantum Bilgisayarları



REVIEWS OF MODERN PHYSICS, VOLUME 92, JANUARY–MARCH 2020

Quantum computational chemistry

Sam McArdle[✉] and Suguru Endo[✉]

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Simon C. Benjamin[✉] and Xiao Yuan^{✉†}

Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

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Fin

