Quantum Journal Club

Place:

Zulip Workspace:
https://zulip.hkust-gz.edu.cn,
Stream: Journal Club-Quantum

Workflow:

1. **Before Friday**: Suggest papers in the topic: **Papers**
2. Friday: Vote for the most interested paper
3. Tuesday: Food ordering
4. Wednesday: Presenting

All presenters: AMAT 5996 final score +10
End of semester: Best presenter award

Presenter’s Guide

- **Choose a good paper**: The topic is usually a recent progress in your field
  - Good example: The First Room-Temperature Ambient-Pressure Superconductor
  - Bad example: Relativity: The Special and General Theory
- **Prepare well**: If your paper is voted as the most interested one, please take at least 1 day to prepare for it. You can present with either **slides** or **whiteboard**.
- **Present like an expert**: Include an overview of your field to help audiences understand the general idea, rather than sticking to some technical details

Many thanks to

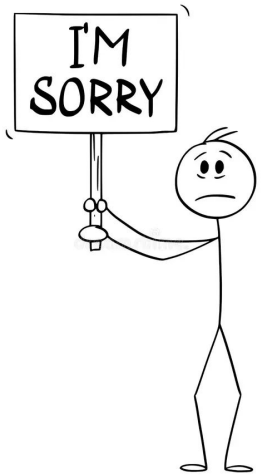
Advanced material thrust (especially Prof. Ping Gao and Ina Guo) for spending over 50% of the total entertainment funding for providing free lunch.

Pan Zhou for ordering the food.

Qing-Yun Qian for agreeing to organize the future events.

Be brave!

Please do not get too frustrated if you can not present well at the beginning, since you audiences at least get free food!



This is the reason why I did not prepare for the journal club topic “Electronic Transport in DNA” this time.

Electronic Transport in DNA

Jinguo Liu

I will share these slides in Zulip

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PHYSICAL REVIEW B, VOLUME 65, 241314(R)

Backbone-induced semiconducting behavior in short DNA wires

Gianaurelio Cuniberti,[1,*] Luis Craco,[1] Danny Porath,[2] and Cees Dekker[3]
[1]*Max Planck Institute for Physics of Complex Systems, D-01187 Dresden, Germany*
[2]*The Physical Chemistry Department, The Hebrew University of Jerusalem, IL-91904 Jerusalem, Israel*
[3]*Department of Applied Physics, Delft University of Technology, NL-2628 CJ Delft, The Netherlands*
(Received 4 March 2002; published 24 June 2002)

We propose a model Hamiltonian for describing charge transport through short homogeneous double stranded DNA molecules. We show that the hybridization of the overlapping π orbitals in the base-pair stack coupled to the backbone is sufficient to predict the existence of a gap in the nonequilibrium current-voltage characteristics with a minimal number of parameters. Our results are in a good agreement with the recent finding of semiconducting behavior in short poly(G)-poly(C) DNA oligomers. In particular, our model provides a correct description of the molecular resonances which determine the quasilinear part of the current out of the gap region.

DOI: 10.1103/PhysRevB.65.241314 PACS number(s): 72.80.Le, 05.60.−k, 87.10.+e, 87.14.Gg

Old papers are not recommended

Biophysical Journal Volume 89 October 2005 2187–2198

Electronic Transport in DNA

Daphne Klotsa, Rudolf A. Römer, and Matthew S. Turner
Physics Department and Centre for Scientific Computing, University of Warwick, Coventry, United Kingdom

ABSTRACT We study the electronic properties of DNA by way of a tight-binding model applied to four particular DNA sequences. The charge transfer properties are presented in terms of localization lengths (crudely speaking, the length over which electrons travel). Various types of disorder, including random potentials, are employed to account for different real environments. We have performed calculations on poly(dG)-poly(dC), telomeric-DNA, random-ATGC DNA, and λ-DNA. We find that random and λ-DNA have localization lengths allowing for electron motion among a few dozen basepairs only. A novel enhancement of localization lengths is observed at particular energies for an increasing binary backbone disorder. We comment on the possible biological relevance of sequence-dependent charge transfer in DNA.

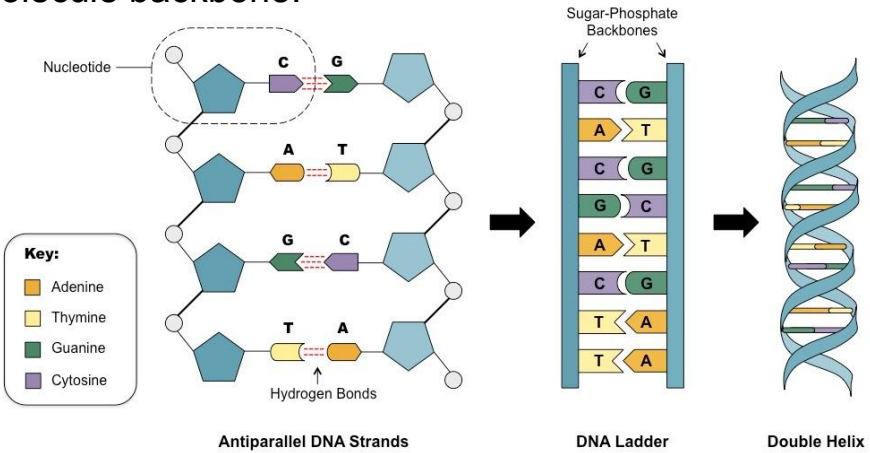
Why electronic transport in DNA?

From biophysicists' perspective: Processes that possibly use electron transfer include the function of DNA damage response enzymes, transcription factors, or polymerase co-factors…

From a quantum information scientist's perspective: Electronic transport properties of DNA may be used for building computing devices. So far, only structural degree of freedoms are used, mainly as a future data storage.

We know so little about electronic properties of DNA

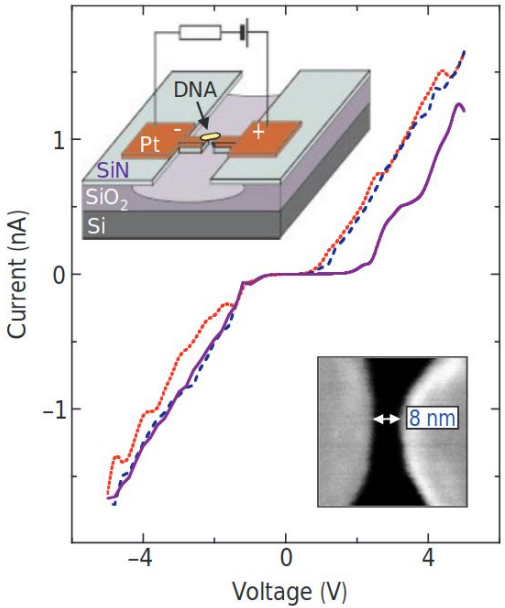
Sugar and phosphate groups forming the molecule backbone.



In its natural environment, DNA is always in liquid solution, and therefore, experimentally, one can study the molecule either in solution or in artificially imposed **dry** environments.

DNA has been reported to be an **insulator**, an Ohmic **conductor**, and a **semiconductor**.

Electrical transport in DNA

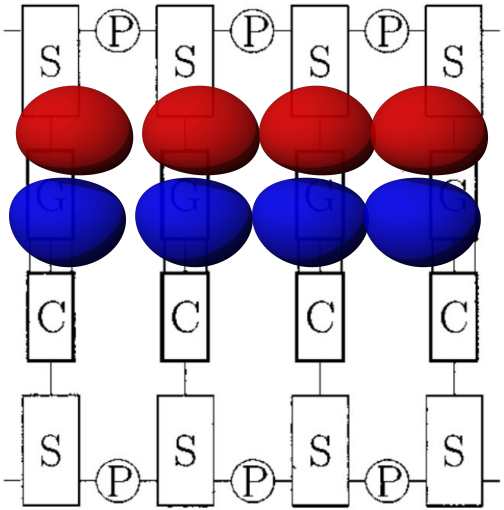


In this chain with 30 G-C pairs forms a semi-conductor

Porath D, Bezryadin A, De Vries S, et al. Direct measurement of electrical transport through DNA molecules[J]. Nature, 2000, 403(6770): 635-638.

Density functional theory is the most accurate, but… very slow

Density-functional calculations have shown that the bases, especially **Guanine**, are rich in p-orbitals.



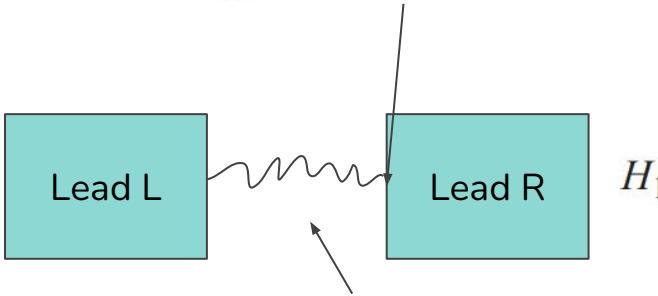
G-G π orbital stack

drawing. In most models of electronic transport (12,37), it has been assumed—following the pioneering work reported in Bakshi et al. (38) and Ladik et al. (39)—that the transmission channels are along the long axis of the DNA molecule (we note that Walet and Zakrzewski (40) assume transport is via the sugar-phosphate backbone), and that the conduction path is due to π-orbital overlap between consecutive bases (17); density-functional calculations (41) have shown that the bases, especially Guanine, are rich in π-orbitals. Quantum mechanical approaches to the problem mostly use strictly one-dimensional tight-binding models (27–31).

Model

$$H = H_{\text{mol}} + H_{\text{leads}} + H_{\text{coupl}}$$

$$H_{\text{coupl}} = -\sum_{\mathbf{k},\sigma} U_{\mathbf{k}} (a^{\dagger}_{\mathbf{k}\sigma \text{L}} b_{1\sigma} + a^{\dagger}_{\mathbf{k}\sigma \text{R}} b_{N\sigma} + \text{H.c.}).$$

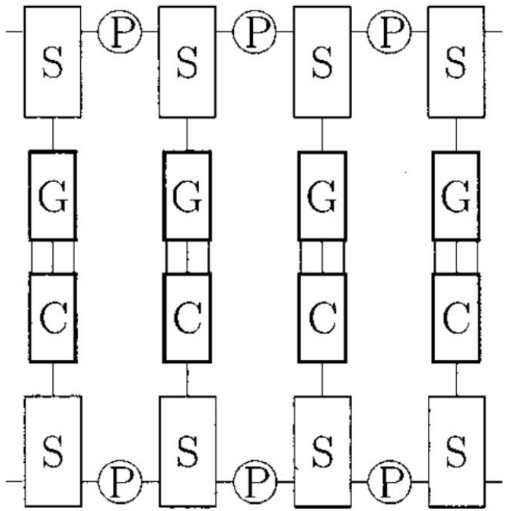


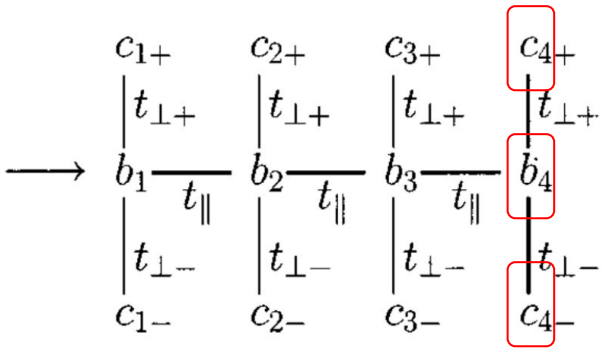
$$H_{\text{leads}} = \sum_{\mathbf{k},\sigma,\nu=\text{L},R} \varepsilon_{\mathbf{k}\nu} a^{\dagger}_{\mathbf{k}\sigma\nu} a_{\mathbf{k}\sigma\nu},$$

The density of electrons at momentum k. We usually use the flat band approximation, i.e. densities are uniform

Left and right are different by a chemical potential

Model - Relevant bands



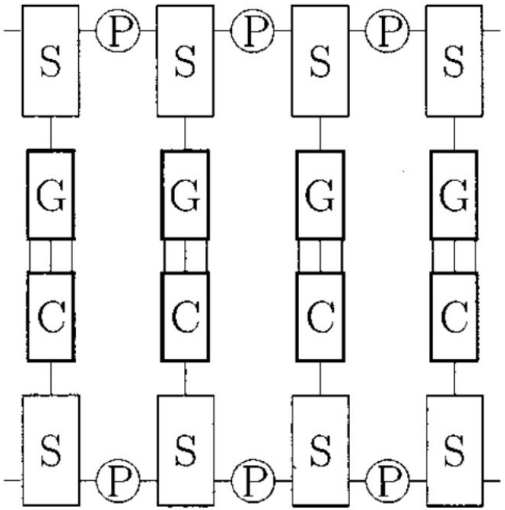


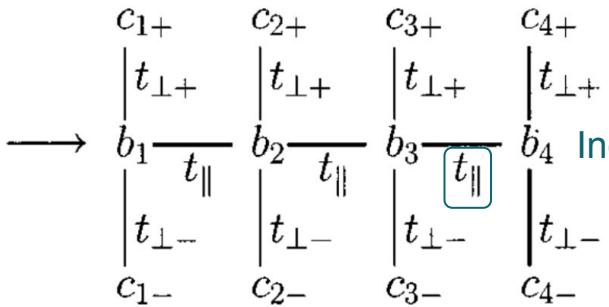
Annihilation operator for upper edge

Annihilation operator for charges with spin σ at G base site i

Annihilation operator for lower edge

G-C DNA chain



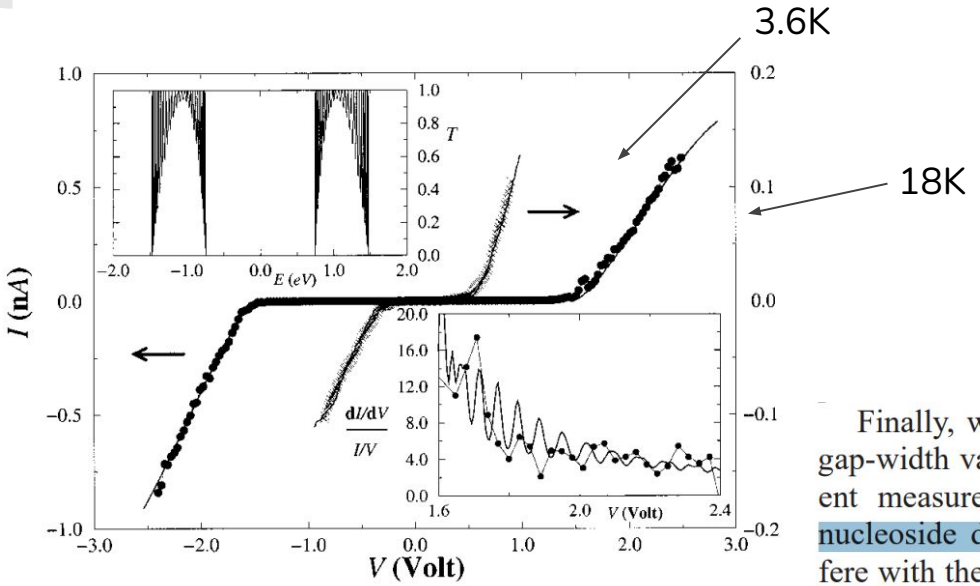


Induced by the G-G π orbital stack

$$H_{\mathrm{mol}} = \varepsilon_b \sum_{i,\sigma} b^{\dagger}_{i\sigma} b_{i\sigma} - t_{\parallel} \sum_{\langle i,j\rangle,\sigma} b^{\dagger}_{i\sigma} b_{j\sigma} + \sum_{i,\sigma,\alpha=\pm} \varepsilon_{\alpha} c^{\dagger}_{i\sigma\alpha} c_{i\sigma\alpha}$$

$$- \sum_{i,\sigma,\alpha=\pm} t_{\perp\alpha} (c^{\dagger}_{i\sigma\alpha} b_{i\sigma} + \mathrm{H.c.}),$$

Result



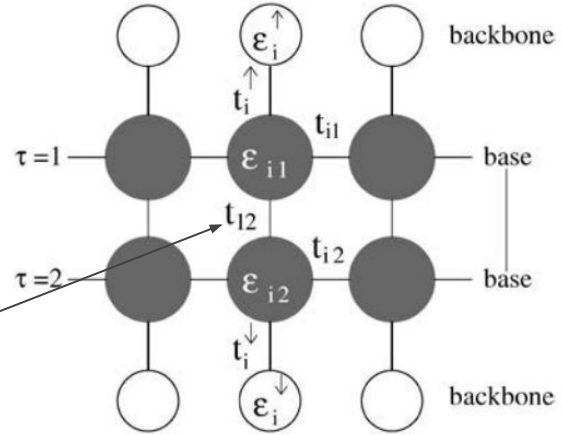
Assumption: $t_{\perp +} = t_{\perp -}$
$t_{//}$ and $t_{\perp}$ are fitted

Method: nonequilibrium Green-function calculations (Keldysh formalism)

Finally, we would also like to comment on the observed gap-width variability, even within the same sample at different measurement sweeps. A structural fluctuation in the nucleoside distribution along the double helix[31] may interfere with the π stack[32] leading to a recalibration of the overlap integrals that indeed drives the gap width and induces a sharp change of the I-V profile. Moreover, the measurement process itself may induce structural rearrangement of the double helix. The strong electric field associated with the

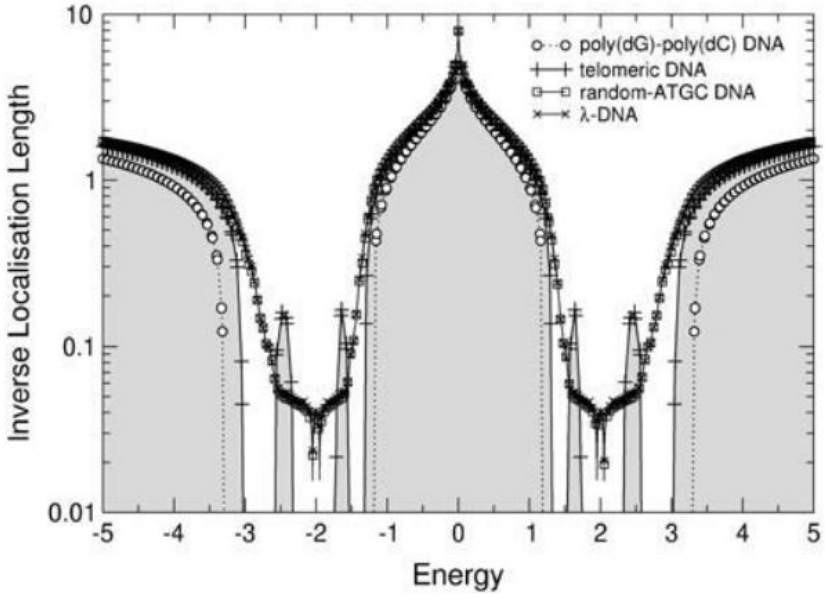
The ladder model

only. The reduction of the DNA basepair architecture into a single site per pair, as in the fishbone model (Eq. 1), is obviously a highly simplified approach. As an improvement on this, we model each base as a distinct site where the basepair is then weakly coupled by the hydrogen bonds. The resulting two-channel model is shown in Fig. 3. This ladder model is a



i.e., perpendicular to the direction of conduction. SPARTAN results suggest that this value—dominated by the wave function and overlapping across the hydrogen bonds—is weak, and so we choose $t_{12} = 1/10$. As before, we also set $\varepsilon_{i,\tau} = 0$ for all i and τ.

Localization



The fishbone and ladder models studied in this article give qualitatively similar results, i.e., a gap in the DOS on the order of the hopping energies to the backbone, extended states for periodic DNA sequences, and localized states for any non-zero disorder strength. Thus, at $T = 0$, our results suggest that DNA is an insulator unless perfectly ordered. Quantitatively, the localization lengths ξ computed for the ladder model are larger than for the fishbone model. Since we are interested in these nonuniversal lengths, the ladder model is clearly the more appropriate model.

Anderson Localization

1D : all states are localized (with infinitesimal disorder)

2D : all states are localized ; the length scale of localization grows exponentially with E and marginal dimension for the Anderson transition