Nonequilibrium Materials Engineering

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Max Planck Institute for the Structure and Dynamics of Matter
Quantum materials

W. Hu et al., Nature Materials 13, 705 (2014)


Image Credit: Department of Theoretical Physics at Ural University
Engineering materials with light

condensed matter
quantum materials
atomic-scale control

ultrafast spectroscopy
revealing elementary couplings
light-induced new states of matter

nonequilibrium
materials engineering

pump-probe: strong classical fields

quantum optics
nanoplasmonics
polaritonic chemistry
QED: vacuum fluctuations

Y. Cao et al., Nature 556, 43 (2018)

R. Chikkaraddy et al., Nature 535, 127 (2016)

Y. Cao et al., Nature 556, 43 (2018)

QED: vacuum fluctuations

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Engineering materials with light

Hamiltonian engineering
e.g., Floquet-Bloch bands

Distributional engineering

many ingredients, hard to disentangle


J. Sobota et al., JESRP 195, 249 (2014)
Engineering materials with light

Exposing hidden states
nonthermal switching process

Light-induced new states
transient superconductivity?

\(1\text{T-TaS}_2\)

Resistance after a laser pulse

\(35\text{ fs (800 nm)}\)

L. Stojchevska et al., Science 344, 177 (2014)

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microscopic understanding?

M. Mitrano et al., Nature 530, 461 (2016)

Igor Vaskivskyi

L. Stojchevska et al., Science 2014;344:177-180

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Pump-probe spectroscopy

- stroboscopic investigations of dynamic phenomena

*Muybridge 1887*

*Image courtesy: J. Sobota / F. Schmitt*
Understanding the nature of quasiparticles
- Relaxation dynamics
- Control of couplings

PRX 3, 041033 (2013)  PRB 95, 205111 (2017)

Understanding ordered phases
- Collective oscillations
- Competing orders

PRB 93, 144506 (2016)  arXiv:1808.00712
arXiv:1810.06536

Creating new states of matter
- nonequilibrium topological states

Nature Comm. 6, 7047 (2015)
Nature Comm. 8, 13940 (2017)
Nature Comm. 9, 4452 (2018)
Electron-boson coupling

Holstein model (minimal version):

\[ H = \sum_k \epsilon(k) c_k^\dagger c_k + \Omega \sum_i b_i^\dagger b_i - g \sum_i c_i^\dagger c_i (b_i + b_i^\dagger) \]

Electrons (Fermi gas/liquid) \hspace{1cm} Bosons (e.g., Einstein phonon) \hspace{1cm} Electron-boson coupling

Pump laser:

\[ \epsilon(k) \rightarrow \epsilon(k, t) \]
Method: Keldysh Green functions

\[ G_k(\omega) = G_k^0(\omega) + G_k^0(\omega) \Sigma(\omega) G_k(\omega) \]

\[ G_k(t, t') = G_k^0(t, t') + \int dt_1 dt_2 G_k^0(t, t_1) \Sigma(t_1, t_2) G_k(t_2, t') \]

self-energy \( \Sigma \):
- electron-electron scattering
- electron-phonon scattering

pump-probe photoemission
Electron-boson coupling

Weak pump

Strong pump

t = -65.00

time unit = 0.66 fs

Rameau et al., Nat. Comm. 7, 13761 (2016)

boson window effect for fast versus slow relaxation

nonlinear response for strong pump
Ordered phases

**PRB 92, 224517 (2015)**

**Higgs amplitude mode oscillations in pump-probe photoemission spectroscopy**

(many others: Murakami, Eckstein, Werner, Knap, Demler, Thorwart, Mitra, Kennes, Millis, ...)

**PRB 93, 144506 (2016)**

**Light-enhanced superconductivity:**
electron-phonon scattering versus collective order parameter dynamics

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Some recent key results

How to engineer materials with light?

Part I: Optical control of chiral superconductors

Short laser pulses allow for switching of Majorana modes

*M. Claassen et al., arXiv:1810.06536*

Part II: From classical to quantized photon fields

Materials engineering in an optical cavity using vacuum fluctuations

*M. A. Sentef et al., Science Advances 4, eaau6969 (2018)*
I Optical control of Majoranas

• prior work: optical control of competing orders

Theory of Laser-Controlled Competing Superconducting and Charge Orders

M. A. Sentef, A. Tokuno, A. Georges, and C. Kollath
Phys. Rev. Lett. 118, 087002 – Published 21 February 2017

– near-resonant laser driving switches between phases

charge-density wave

s-wave superconductor
I Optical control of Majoranas

• can one switch the chirality of a 2D topological superconductor?

Sr$_2$RuO$_4$, highly doped graphene, twisted bilayer graphene, ...?

key idea: use two-pulse sequence with linearly and circularly polarized light
Nonequilibrium pathway to switching

\[ \Delta_{\text{equilibrium}} \sim \begin{cases} p_x + i p_y \\ p_x - i p_y \end{cases} \]

\[ \Delta_{\text{non-eq}}(t) \sim \cos(\theta) \ "p_x + i p_y" + \sin(\theta) e^{i \phi} \ "p_x - i p_y" \]
multiband Bogoliubov-de-Gennes Hamiltonians for doped graphene (d+id) and Sr$_2$RuO$_4$ (p+ip) coupling to fermionic reservoir to dissipate energy

laser driving via Peierls substitution

self-consistent Keldysh equations of motion for Nambu Green’s functions:
Optical control of Majoranas

two-pulse sequence reverses d+id state in graphene

time-resolved spectroscopy tracks chirality reversal
Bloch vector rotation
A “programmable” topological quantum computer?

**non-Abelian statistics of Majorana fermions:**
- half-quantum vortices of chiral superconductors host single Majorana fermions
- Two Majoranas represent one electron: $\frac{1}{2} + \frac{1}{2} = 1$

→ Braiding between Majoranas is a non-Abelian operation in electron (charge) basis!

simplest operation: a **switchable Hadamard gate**

Ivanov, PRL 86, 268 (2001)
B. Lian et al., PNAS 115, 10938 (2018)
Summary I

- All-optical control of chiral Majorana modes
- towards arbitrarily programmable quantum computer?

“program the gate optically, read it out electrically“


M. Claassen  D. Kennes
From classical to quantum light

collective strong light-matter coupling

what about cavity materials?

R. Chikkaraddy et al., Nature 535, 127 (2016)
II Cavity materials

- can one use enhanced vacuum fluctuations to change materials properties?
Cavity materials

**BCS superconductors:** phonon-mediated superconductivity


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**Cavity-assisted mesoscopic transport of fermions:**

Coherent and dissipative dynamics.

*Hagenmüller et al., 1801.09876*

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**Cavity-mediated electron-photon superconductivity**

Frank Schlawin, Andrea Cavalleri, and Dieter Jaksch

*1804.07142*

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**Cavity Quantum Eliashberg Enhancement of Superconductivity**

Jonathan B. Curtis, Zachary M. Raines, Andrew A. Allocco, Mohammad Hafezi, and Victor M. Galitski

*1805.01482*

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**Manipulating quantum materials with quantum light**

Martin Kifner, Jonathan Coulthard, Frank Schlawin, Arzhang Ardavan, and Dieter Jaksch

*1806.06752*

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**Cavity superconductor-polaritons**

Andrew A. Allocco, Zachary M. Raines, Jonathan B. Curtis, and Victor M. Galitski

*1807.06601*

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**Superradiant Quantum Materials**

Giacomo Mazza and Antoine Georges

*1804.08534*

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**Ab-initio Exciton-polaritons:**

Cavity control of Dark Excitons in two dimensional Materials

Simone Latini, Enrico Ronca, Umberto De Giovannini, Hannes Hüttener, and Angel Rubio

*1810.02672*
monolayer FeSe/STO: $T_c > 65$ K
bulk FeSe: $T_c = 9$ K

monolayer FeSe/STO: ARPES

experiment

theory

replica bands: forward (small-q) electron-phonon scattering

Lee et al., Nature 515, 245 (2014)

Rademaker et al., New J. Phys. 18, 022001 (2016)
monolayer FeSe/STO: interfacial phonon

bare el-phonon vertex

\[ g(q) = g_0 \exp\left(-\frac{|q|}{q_0}\right) \]

\[ q_0^{-1} = \hbar_0 \sqrt{\epsilon_{||}/\epsilon_\perp} \]

\[ \epsilon_{||}/\epsilon_\perp \approx 100 \]

Lee et al., Nature 515, 245 (2014)

Huang and Hoffman, Annu. Rev. CMP 8, 311 (2017)
Cavity engineering

- idea: use **phonon polaritons** to enhance electron-phonon coupling

_Huang and Hoffman, Annu. Rev. CMP 8, 311 (2017)_
Model and Method

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$$H = \sum_{\vec{k},\sigma} \epsilon_{k} c_{k,\sigma}^{\dagger} c_{k,\sigma} + \frac{1}{\sqrt{N}} \sum_{\vec{k}, \vec{q}, \sigma, \lambda=\pm} c_{\vec{k}+\vec{q},\sigma}^{\dagger} c_{\vec{k},\sigma} (g_{\lambda}^{*}(\vec{q}) \alpha^{\dagger}_{-\vec{q},\lambda} + g_{\lambda}(\vec{q}) \alpha_{\vec{q},\lambda}) + \sum_{\vec{q}, \lambda=\pm} \omega_{\lambda}(\vec{q}) \alpha^{\dagger}_{\vec{q},\lambda} \alpha_{\vec{q},\lambda}$$

G-self-consistent Migdal-Eliashberg diagram

$$g(\vec{q}) = g_{0} \exp(-|\vec{q}|/q_{0}) \quad q_{0}^{-1} = h_{0} \sqrt{\epsilon_{||}/\epsilon_{\perp}}$$

$$\hat{\Sigma}(\vec{k}, i\omega_{n}) = \frac{-1}{N\beta} \sum_{\vec{q}, m, \lambda=\pm} |g_{\lambda}(\vec{q})|^{2} D^{(0)}_{\lambda}(\vec{q}, i\omega_{n} - i\omega_{m}) \hat{\tau}_{3} \hat{G}(\vec{k} + \vec{q}, i\omega_{m}) \hat{\tau}_{3}$$

$$\hat{\Sigma}(\vec{k}, i\omega_{n}) = i\omega_{n}[1 - Z(\vec{k}, i\omega_{n})] \hat{\tau}_{0} + \chi(\vec{k}, i\omega_{n}) \hat{\tau}_{3} + \phi(\vec{k}, i\omega_{n}) \hat{\tau}_{1}$$

$$\lambda \equiv Z(\vec{k}_{F}, i\pi/\beta) - 1$$

Mass enhancement: $$m^*/m = 1 + \lambda$$
Cavity materials: Phonon polaritons

\[ \omega(q) \]

- \( \omega_+ \) (upper polariton)
- \( \omega_- \) (lower polariton)
- \( \omega \) (photon)
- \( \Delta \) (phonon)

A enhanced electron-phonon coupling, controlled by cavity volume
Suppressed superconductivity despite enhanced el-ph coupling

Forward scattering

$$T_C \approx \frac{\lambda \Omega}{2 + 3\lambda}$$

vs.

$$T_{C,BCS} \approx 1.13\Omega \exp\left(-\frac{1}{\chi}\right)$$

q-independent scattering
• cavity leads to enhanced electron-phonon coupling
• can one also enhance superconductivity?

Science Advances 4, eaau6969 (2018)
Team and collaborators

thank you for your attention!