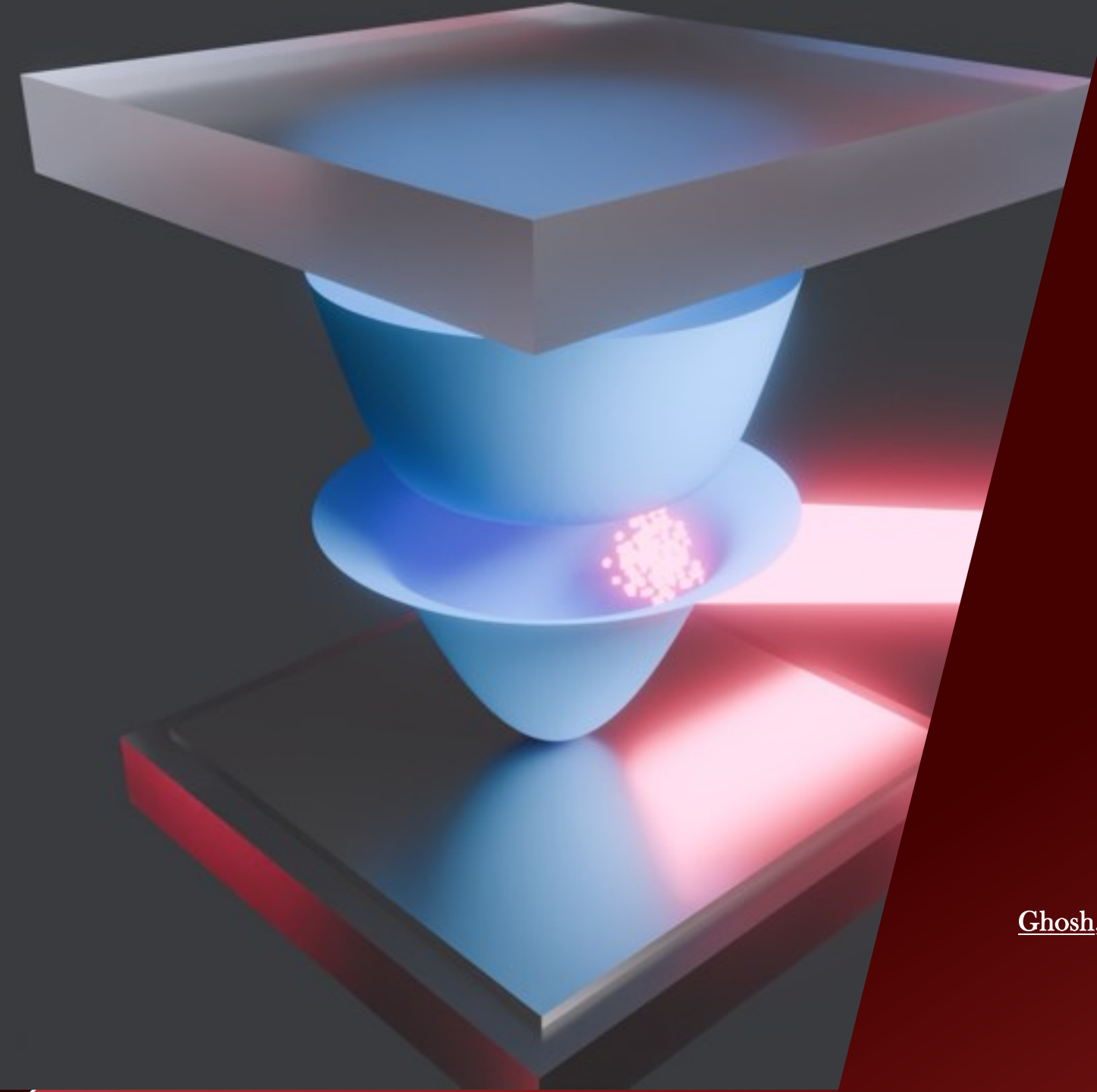


TEXAS A&M UNIVERSITY

Many Body Quantum Dynamics *of* Exciton-Polaritons

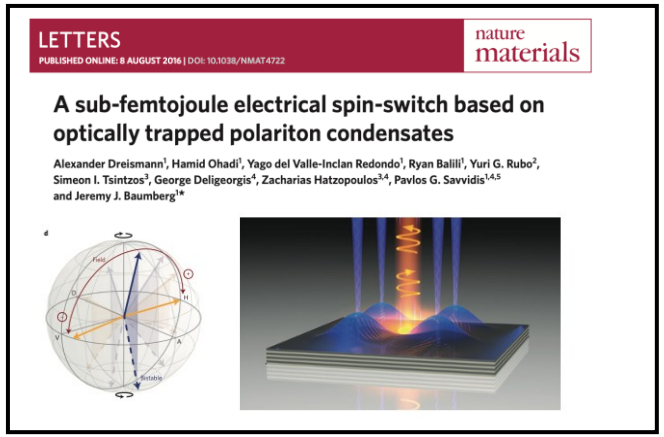
Pritha Ghosh

Mandal Group, *Department of Chemistry*

Ghosh, Manjalingal, Wickramasinghe, Rahmanian, Mandal, Phys. Rev. B. (2025)
Editors' Suggestion

Motivation

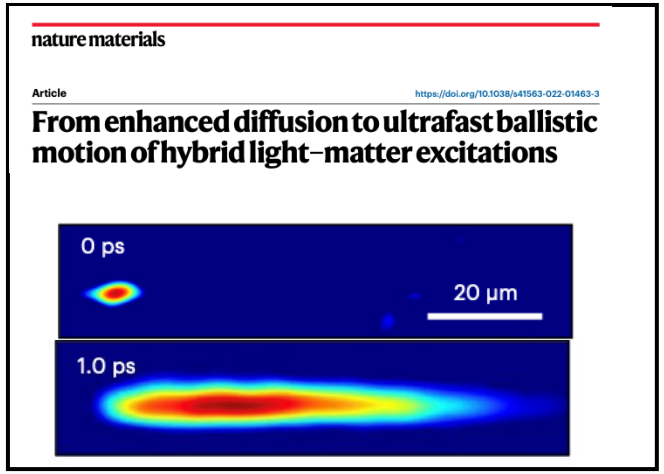
Polaritons Exhibit Room-temperature **Quantum Coherence!**


LETTERS
PUBLISHED ONLINE: 8 AUGUST 2016 | DOI: 10.1038/NMAT4722
nature materials

A sub-femtojoule electrical spin-switch based on optically trapped polariton condensates

Alexander Dreismann[1], Hamid Ohadi[1], Yago del Valle-Inclan Redondo[1], Ryan Balili[1], Yuri G. Rubo[2], Simeon I. Tsintzos[3], George Deligeorgis[4], Zacharias Hatzopoulos[3,4], Pavlos G. Savvidis[1,4,5] and Jeremy J. Baumberg[1]*

Room-temperature Bose-Einstein Condensate.


nature materials

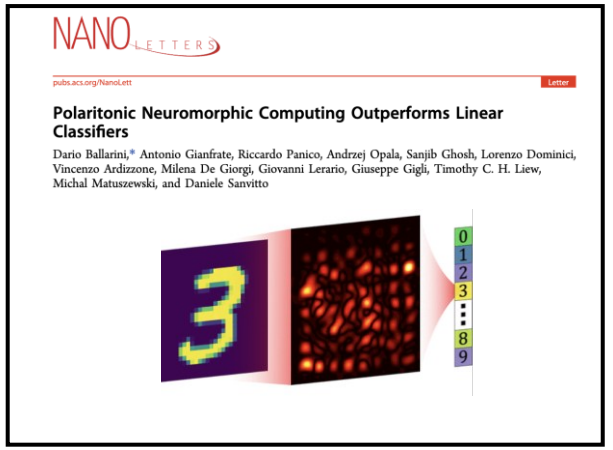
Article https://doi.org/10.1038/s41563-022-01463-3

From enhanced diffusion to ultrafast ballistic motion of hybrid light–matter excitations

0 ps
20 μm
1.0 ps

Room temperature Coherent Propagation of Excitons.

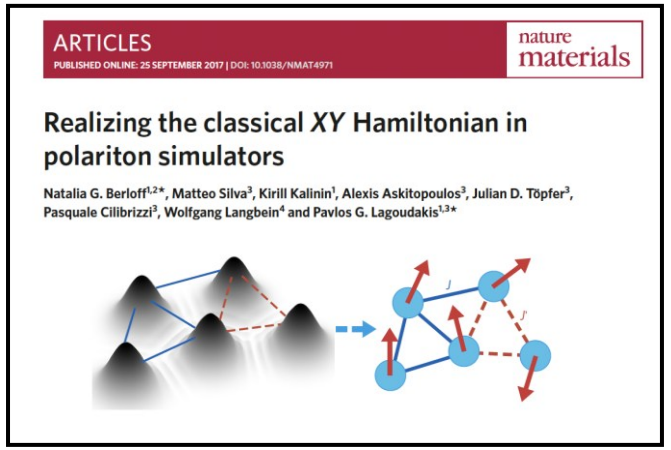
Diverse Applications!


NANO LETTERS
pubs.acs.org/NanoLett Letter

Polaritonic Neuromorphic Computing Outperforms Linear Classifiers

Dario Ballarini,* Antonio Gianfrate, Riccardo Panico, Andrzej Opala, Sanjib Ghosh, Lorenzo Dominici, Vincenzo Ardizzone, Milena De Giorgi, Giovanni Lerario, Giuseppe Gigli, Timothy C. H. Liew, Michal Matuszewski, and Daniele Sanvitto

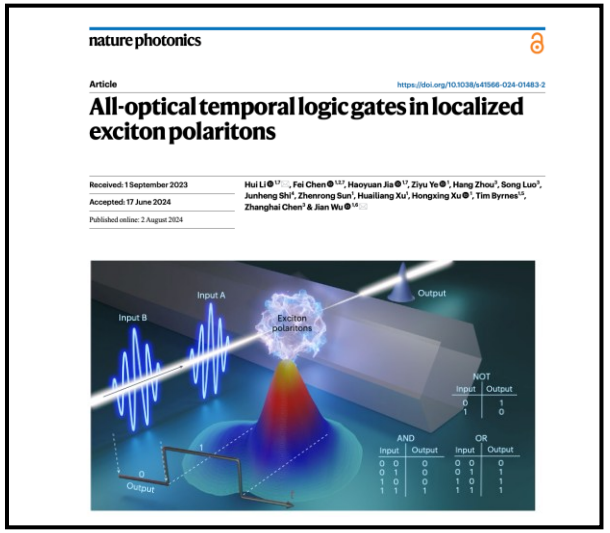
Efficient Neuromorphic Computing


ARTICLES
PUBLISHED ONLINE: 25 SEPTEMBER 2017 | DOI: 10.1038/NMAT4971
nature materials

Realizing the classical *XY* Hamiltonian in polariton simulators

Natalia G. Berloff[1,2]*, Matteo Silva[3], Kirill Kalinin[1], Alexis Askitopoulos[3], Julian D. Töpfer[3], Pasquale Cilibrizzi[3], Wolfgang Langbein[4] and Pavlos G. Lagoudakis[1,3]*

Platform for Analogue Quantum Computing


nature photonics

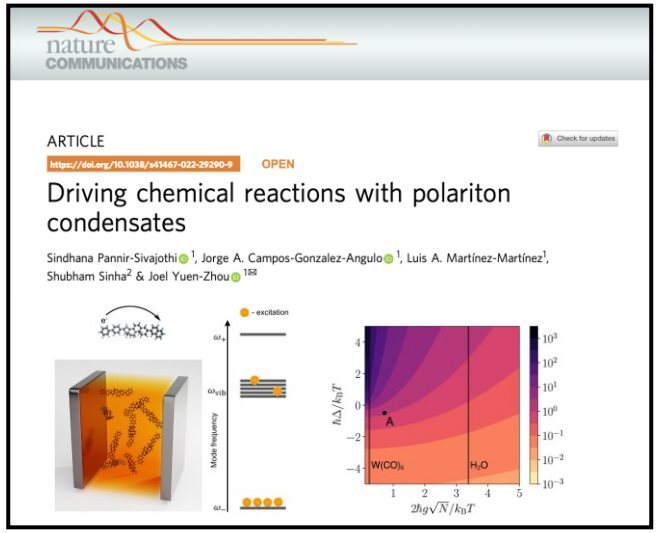
Article https://doi.org/10.1038/s41566-024-01483-2

All-optical temporal logic gates in localized exciton polaritons

Received: 1 September 2023
Accepted: 17 June 2024
Published online: 2 August 2024

Hui Li, Fei Chen, Haoyuan Jia, Ziyu Ye, Hang Zhou, Song Luo, Junheng Shi, Zhenrong Sun, Huailiang Xu, Hongxing Xu, Tim Byrnes, Zhanghai Chen & Jian Wu

Exciton-polariton Based Logic Gates


nature COMMUNICATIONS

ARTICLE
https://doi.org/10.1038/s41467-022-29290-9 OPEN

Driving chemical reactions with polariton condensates

Sindhana Pannir-Sivajothi, Jorge A. Campos-Gonzalez-Angulo, Luis A. Martínez-Martínez, Shubham Sinha & Joel Yuen-Zhou

Exotic Chemistry in Cavities

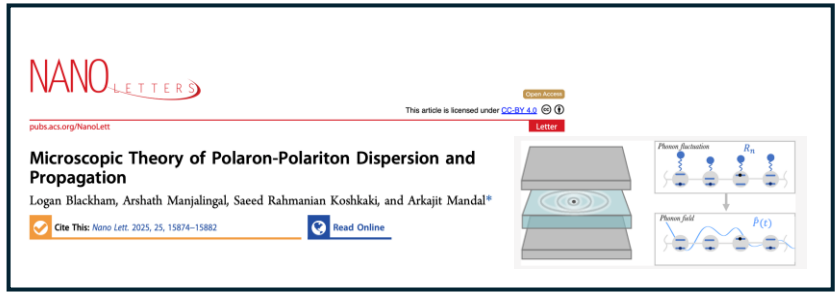
Theoretical Challenges

Holstein Tavis-Cummings


NANO LETTERS

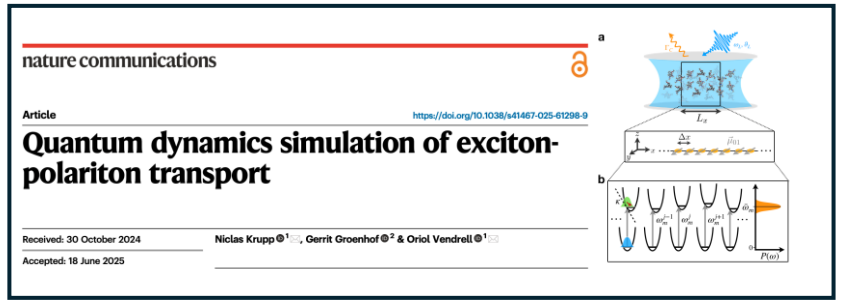
Quantum Dynamics Simulations of Exciton Polariton Transport

Benjamin X. K. Chng, M. Elious Mondal, Wenxiang Ying, and Pengfei Huo*


NANO LETTERS

Microscopic Theory of Polaron-Polariton Dispersion and Propagation

Logan Blackham, Arshath Manjalingal, Saeed Rahmanian Koshkaki, and Arkajit Mandal*


nature communications

Article

Quantum dynamics simulation of exciton-polariton transport

Received: 30 October 2024

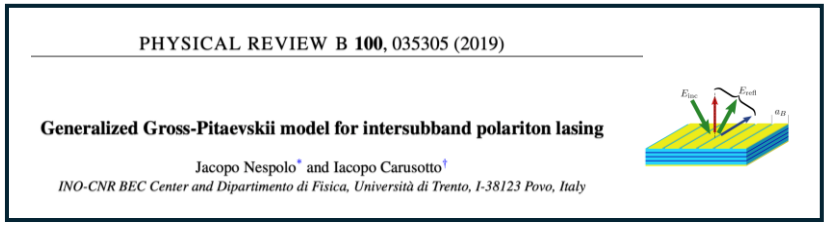
Accepted: 18 June 2025

Niclas Krupp[1], Gerrit Groenhof[2] & Oriol Vendrell[1]

Explicit Phonon Interaction ✓

Many body interactions ✗

Gross-Pitaevskii


PHYSICAL REVIEW B 100, 035305 (2019)

Generalized Gross-Pitaevskii model for intersubband polariton lasing

Jacopo Nespolo* and Iacopo Carusotto†

INO-CNR BEC Center and Dipartimento di Fisica, Università di Trento, I-38123 Povo, Italy

Explicit Phonon Interaction ✗

Many body interactions ✓


IOP Publishing | London Mathematical Society

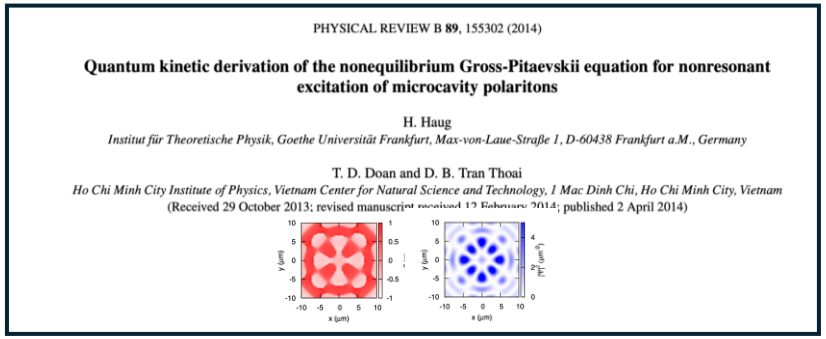
Nonlinearity

Nonlinearity 32 (2019) 4317–4345

https://doi.org/10.1088/1361-6544/ab2bc1

On a dissipative Gross–Pitaevskii-type model for exciton-polariton condensates*

Paolo Antonelli[1], Peter Markowich[2], Ryan Obermeyer[3], Jesus Sierra[4] and Christof Sparber[3]


PHYSICAL REVIEW B 89, 155302 (2014)

Quantum kinetic derivation of the nonequilibrium Gross-Pitaevskii equation for nonresonant excitation of microcavity polaritons

H. Haug

Institut für Theoretische Physik, Goethe Universität Frankfurt, Max-von-Laue-Straße 1, D-60438 Frankfurt a.M., Germany

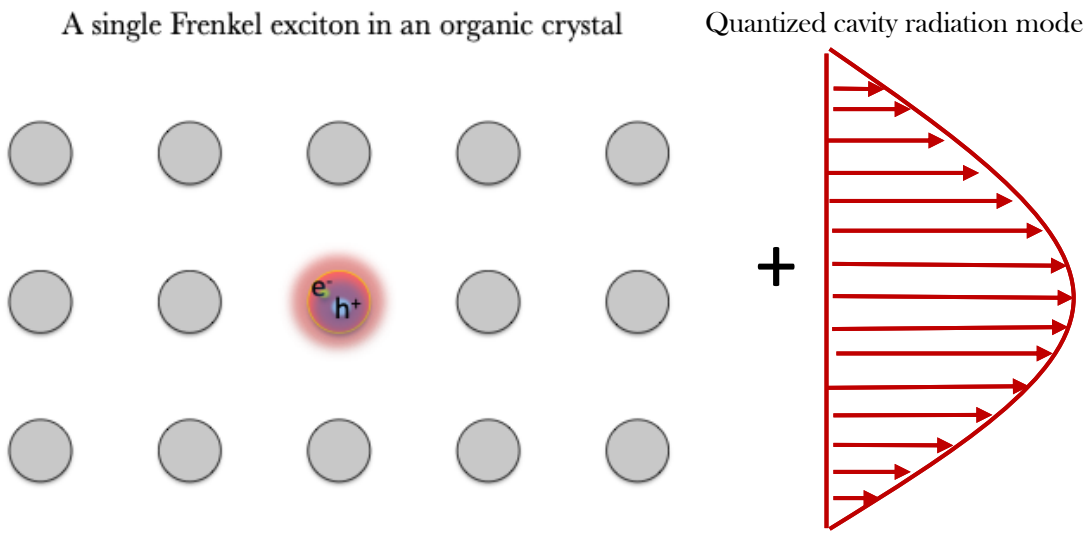
T. D. Doan and D. B. Tran Thoai

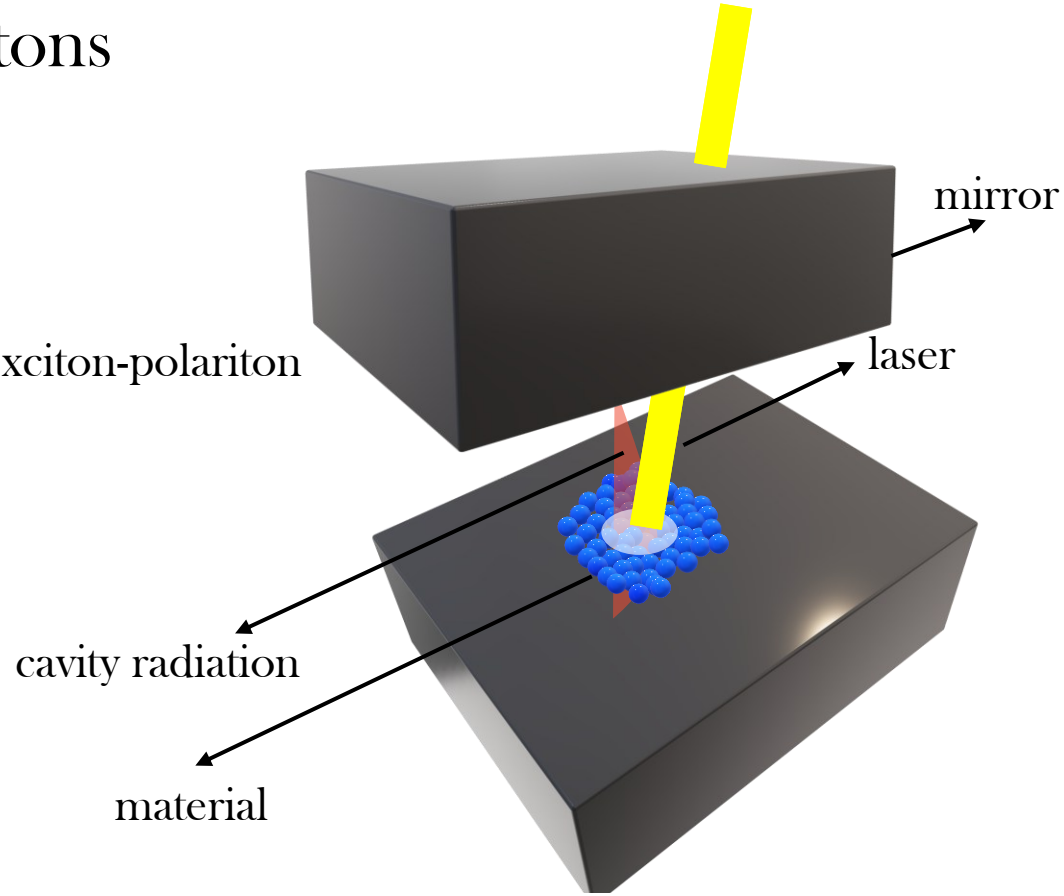
Ho Chi Minh City Institute of Physics, Vietnam Center for Natural Science and Technology, 1 Mac Dinh Chi, Ho Chi Minh City, Vietnam

(Received 29 October 2013; revised manuscript received 12 February 2014; published 2 April 2014)

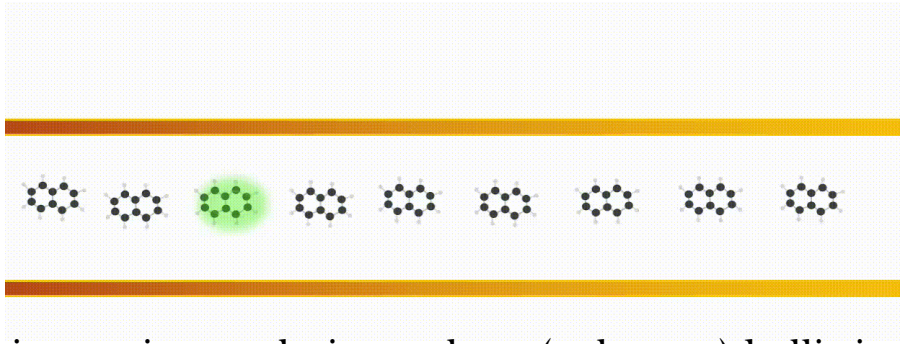
Simulating polaritons at room temperature → Mesoscale systems + many-body interactions + coupling to phonons

Exciton-polaritons



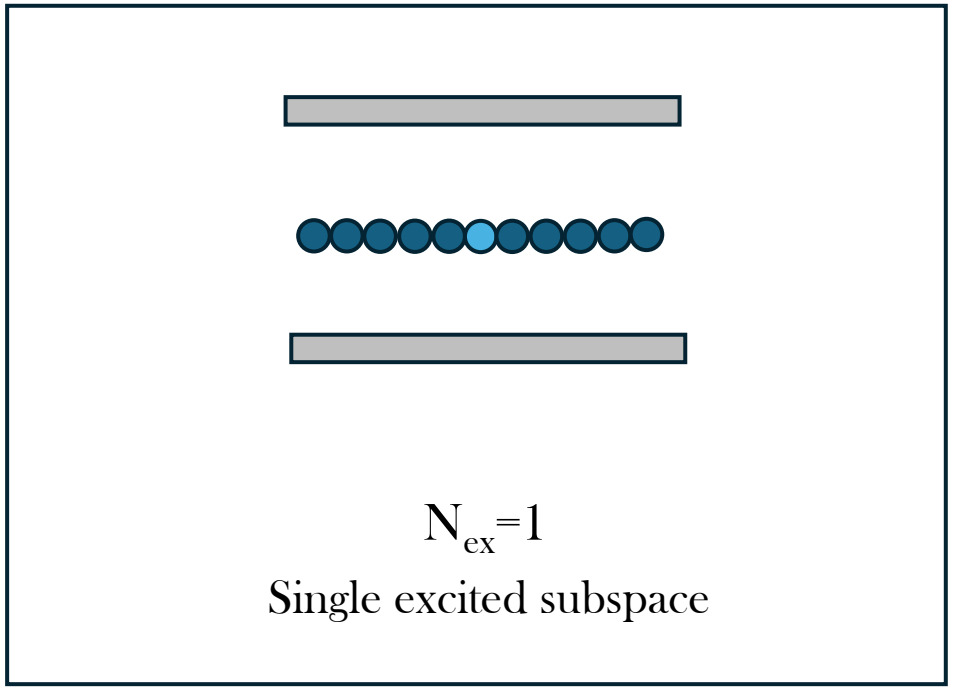


In a bare material, exciton shows (incoherent) diffusive transport.



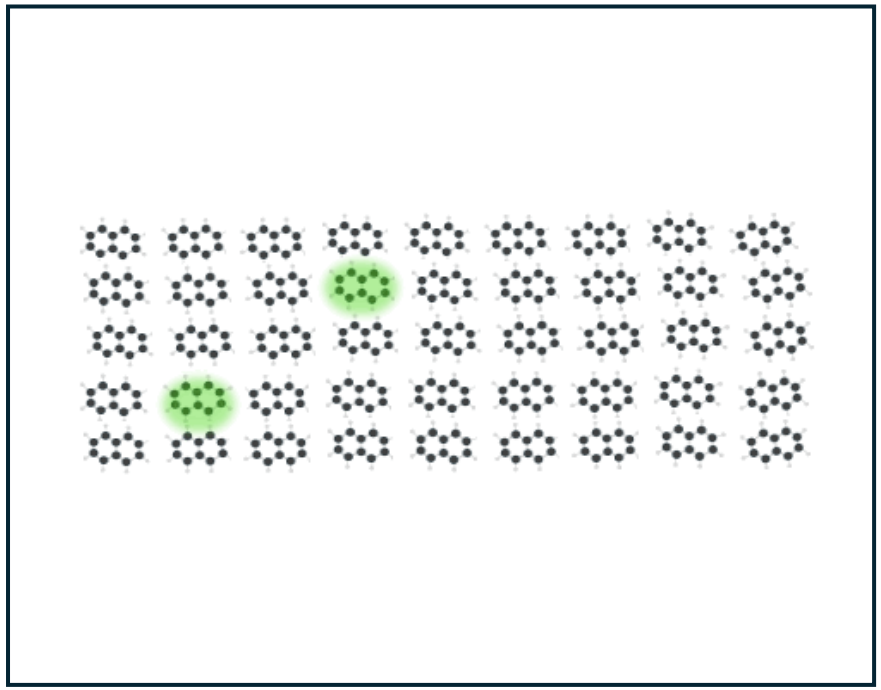
In a cavity, exciton-polaritons show (coherent) ballistic transport.

INCOMPATIBLE with experiments!

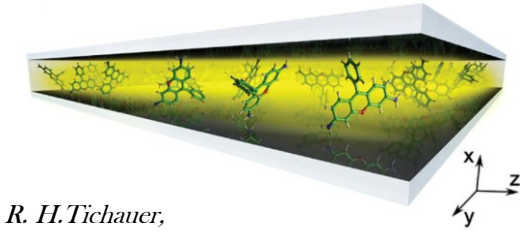


$N_{ex}=1$

Single excited subspace

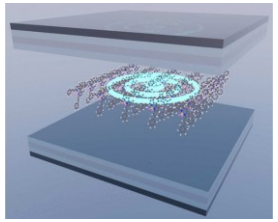


For Nex>>1, many-body interactions have to be included → dynamics become **complicated**!



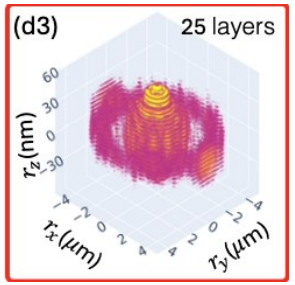
R. H. Tichauer, I.Sokolovskii, G.Groenhof,. Adv. Sci. 2023

~500 molecules



Chng, Nano Lett. 2025

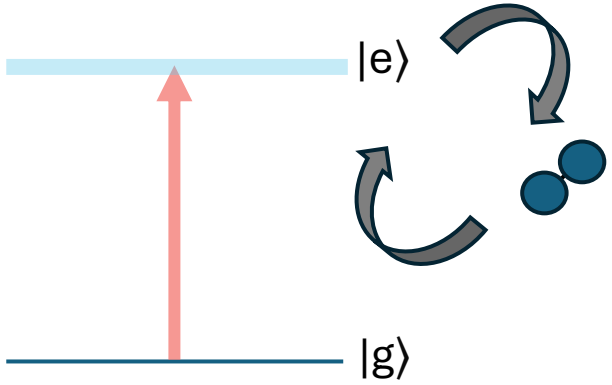
~10^4 molecules



Koshkaki, arXiv:2502.12933v2

>10^6 molecules

Mixed quantum classical simulation



Multitrajectory Ehrenfest

Fewest Switches Surface Hopping

Path Integral Based Approach

Huge numbers of classical degrees of freedom

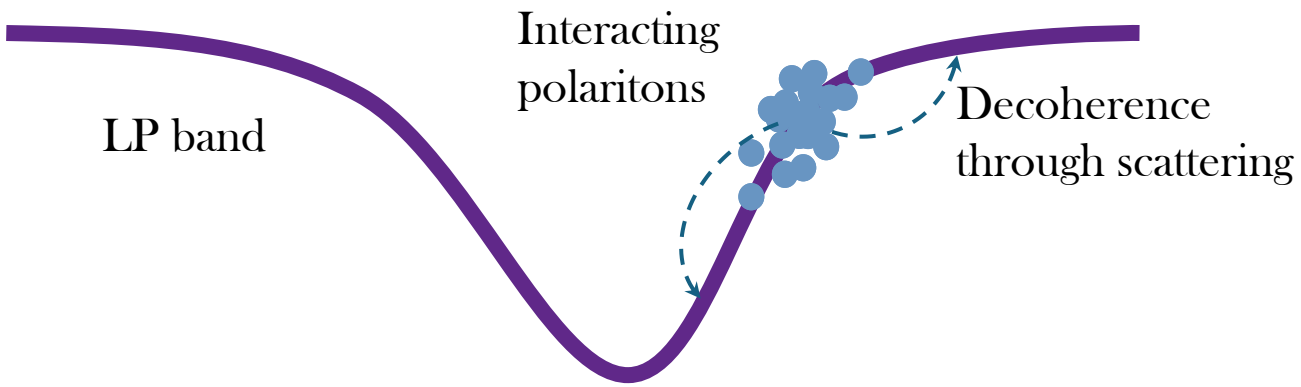
Computationally intractable!

A **novel** approach

Multitrajectory mean field Ehrenfest for the phonons (quasi-classical)

+

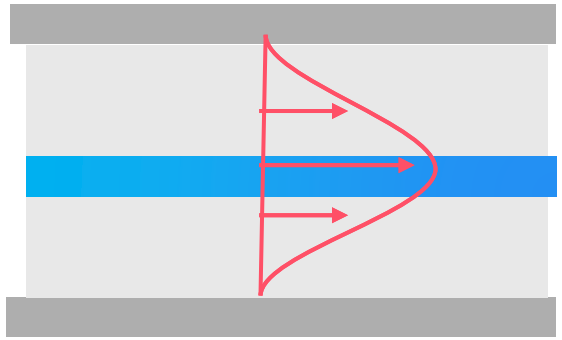
Mean field Gross-Pitaevskii for the exciton-polaritons (quantum)



Light-Matter Hamiltonian

$$\hat{H}_{\mathrm{LM}} = \hat{H}_{\mathrm{e}} + \hat{H}_{\mathrm{p}} + \hat{H}_{\mathrm{e-p}} + \hat{H}_{\mathrm{c}} + \hat{H}_{\mathrm{e-c}}.$$

$$= \sum_{n,m} \epsilon_{n,m} \hat{X}_n^\dagger \hat{X}_m + \frac{U}{2} \sum_n \hat{X}_n^\dagger \hat{X}_n^\dagger \hat{X}_n \hat{X}_n + \sum_n \frac{\hat{P}_n^2}{2} + \frac{1}{2}\omega^2 \hat{R}_n^2 + \gamma \sum_n \hat{X}_n^\dagger \hat{X}_n \hat{R}_n + \sum_k \hat{a}_k^\dagger \hat{a}_k \omega_k + \sum_{n,k} \frac{\Omega_k}{\sqrt{N}} \left[\hat{a}_k^\dagger \hat{X}_n e^{-ik\cdot r_n} + \hat{a}_k \hat{X}_n^\dagger e^{ik\cdot r_n} \right].$$



Light-Matter Hamiltonian

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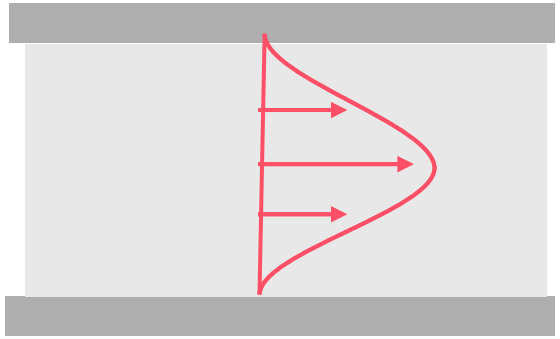
$$= \sum_{n,m} \epsilon_{n,m} \hat{X}_n^\dagger \hat{X}_m + \frac{U}{2} \sum_n \hat{X}_n^\dagger \hat{X}_n^\dagger \hat{X}_n \hat{X}_n + \sum_n \frac{\hat{P}_n^2}{2} + \frac{1}{2}\omega^2 \hat{R}_n^2 + \gamma \sum_n \hat{X}_n^\dagger \hat{X}_n \hat{R}_n + \sum_k \hat{a}_k^\dagger \hat{a}_k \omega_k + \sum_{n,k} \frac{\Omega_k}{\sqrt{N}} \left[\hat{a}_k^\dagger \hat{X}_n e^{-ik\cdot r_n} + \hat{a}_k \hat{X}_n^\dagger e^{ik\cdot r_n} \right].$$

Material
Excitation
(quantum)



Light-Matter Hamiltonian

$$\hat{H}_{\mathrm{LM}} = \hat{H}_{\mathrm{e}} + \hat{H}_{\mathrm{p}} + \hat{H}_{\mathrm{e-p}} + \hat{H}_{\mathrm{c}} + \hat{H}_{\mathrm{e-c}}.$$

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Cavity Photons (quantum)

Light-Matter Hamiltonian

$$\hat{H}_{\mathrm{LM}} = \hat{H}_{\mathrm{e}} + \hat{H}_{\mathrm{p}} + \hat{H}_{\mathrm{e-p}} + \hat{H}_{\mathrm{c}} + \hat{H}_{\mathrm{e-c}}.$$

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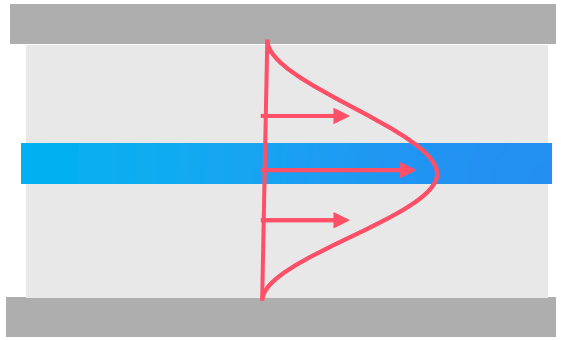
Light Matter Interactions



Light-Matter Hamiltonian

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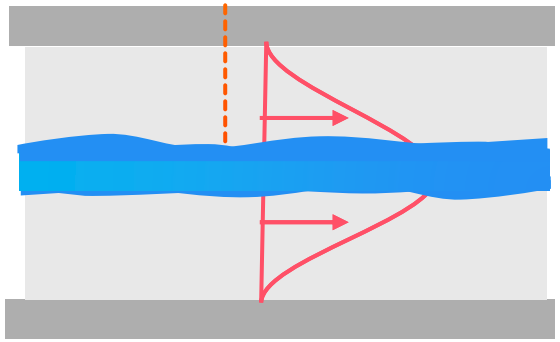
Phonon interactions
(quasi-classical)



Light-Matter Hamiltonian

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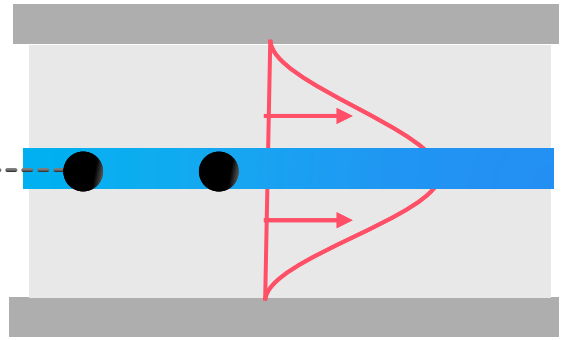
$$= \sum_{n,m} \epsilon_{n,m} \hat{X}_n^\dagger \hat{X}_m + \boxed{\frac{U}{2} \sum_n \hat{X}_n^\dagger \hat{X}_n^\dagger \hat{X}_n \hat{X}_n} + \sum_n \frac{\hat{P}_n^2}{2} + \frac{1}{2}\omega^2 \hat{R}_n^2 + \gamma \sum_n \hat{X}_n^\dagger \hat{X}_n \hat{R}_n + \sum_k \hat{a}_k^\dagger \hat{a}_k \omega_k + \sum_{n,k} \frac{\Omega_k}{\sqrt{N}} \left[\hat{a}_k^\dagger \hat{X}_n e^{-ik\cdot r_n} + \hat{a}_k \hat{X}_n^\dagger e^{ik\cdot r_n} \right].$$

Exciton-Exciton interactions **(on-site)**



Choice of Ansatz

$$\hat{H}_{\mathrm{LM}} = \hat{H}_{\mathrm{e}} + \hat{H}_{\mathrm{p}} + \hat{H}_{\mathrm{e-p}} + \hat{H}_{\mathrm{c}} + \hat{H}_{\mathrm{e-c}}.$$

$$= \sum_{n,m} \epsilon_{n,m} \hat{X}_n^\dagger \hat{X}_m + \frac{U}{2} \sum_n \hat{X}_n^\dagger \hat{X}_n^\dagger \hat{X}_n \hat{X}_n$$

$$+ \sum_n \frac{\hat{P}_n^2}{2} + \frac{1}{2}\omega^2 \hat{R}_n^2 + \gamma \sum_n \hat{X}_n^\dagger \hat{X}_n \hat{R}_n$$

$$+ \sum_k \hat{a}_k^\dagger \hat{a}_k \omega_k + \sum_{n,k} \frac{\Omega_k}{\sqrt{N}} \left[\hat{a}_k^\dagger \hat{X}_n e^{-ik\cdot r_n} + \hat{a}_k \hat{X}_n^\dagger e^{ik\cdot r_n} \right].$$

m=n → on-site energy (ϵ_0)
m ≠ n → hopping (τ)

On- site many body interactions

Mixed Quantum Classical Dynamics

$$\dot{P}_n(t) = -\left\langle \Psi(t) \middle| \frac{\mathrm{d}\hat{H}_{\mathrm{LM}}}{\mathrm{d}R_n} \middle| \Psi(t) \right\rangle, \quad \dot{R}_n(t) = P_n(t)$$

$$i|\dot{\Psi}(t)\rangle = \left[\hat{H}_{\mathrm{LM}} - \frac{1}{2} \sum_n \frac{P_n^2}{2} \right] |\Psi(t)\rangle$$

Intractable

Mean-field Ansatz

$$|\Psi(t)\rangle = \frac{\left(\hat{B}_0^\dagger(t)\right)^{N_{\mathrm{ex}}}}{\sqrt{N_{\mathrm{ex}}!}} |0\rangle.$$

$$B_0^\dagger(t) = \sum_n \psi_n(t) \cdot \hat{X}_n^\dagger + \sum_k \phi_k(t) \cdot \hat{a}_k^\dagger$$

EOM

Finally, using the Dirac-Frenkel Variational Principle,

EOM of the exciton-photon quantum subsystem

$$i\dot{\psi}_n(t) = \epsilon_0\psi_n(t) - \tau(\psi_{n+1}(t) + \psi_{n-1}(t)) + \gamma\psi_n(t)R_n(t) + \sum_k \frac{\Omega_k}{\sqrt{N}}\phi_k(t)e^{-ik\cdot r_n}$$
$$+ U(N_{\text{ex}} - 1)|\psi_n(t)|^2\psi_n(t)$$

$$i\dot{\phi}_k(t) = \phi_k(t)\omega_k + \sum_n \frac{\Omega_k}{\sqrt{N}}\psi_n(t)e^{-ik\cdot r_n}$$

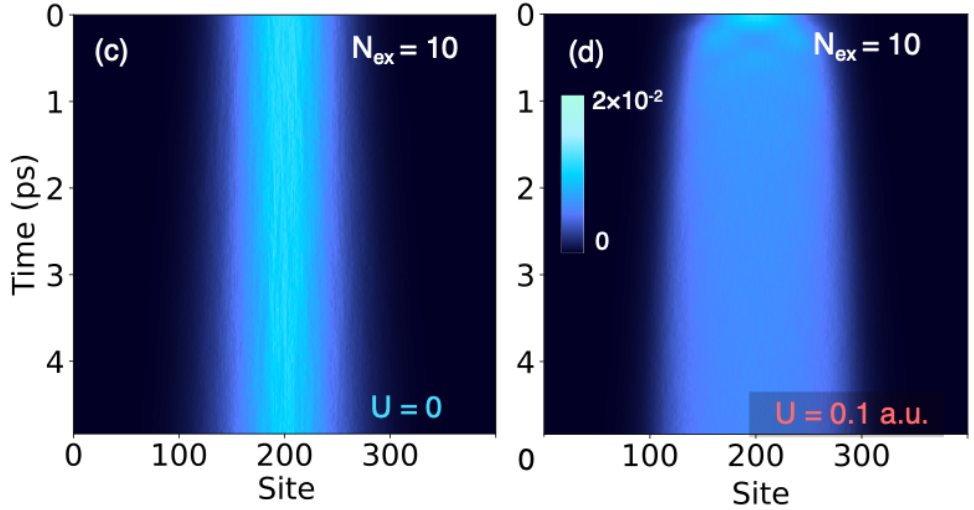
EOM of the phonons

$$\dot{R}_n(t) = P_n(t)$$

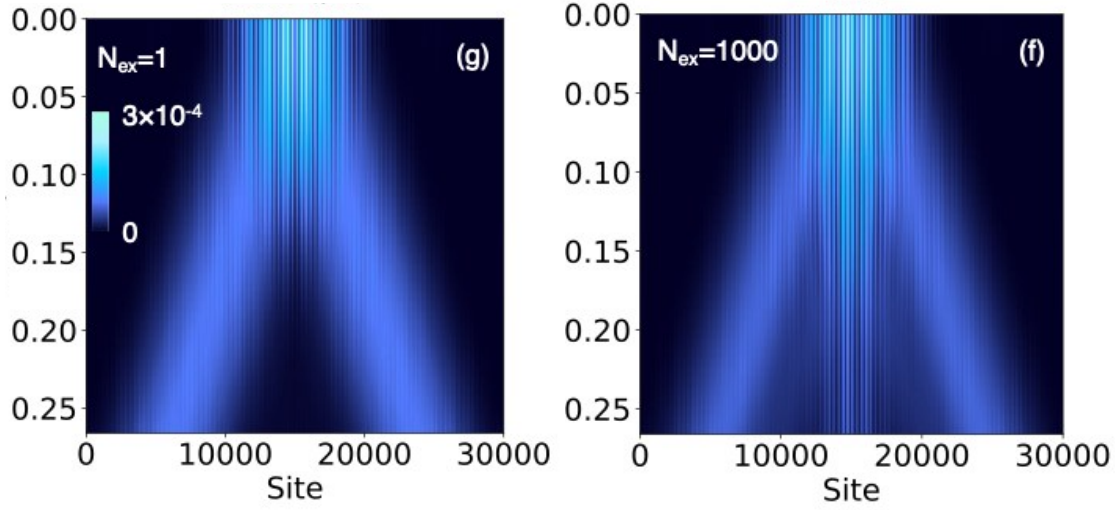
$$\dot{P}_n(t) = -\omega^2 R_n - \gamma|\psi_n(t)|^2 N_{\text{ex}}$$

Results

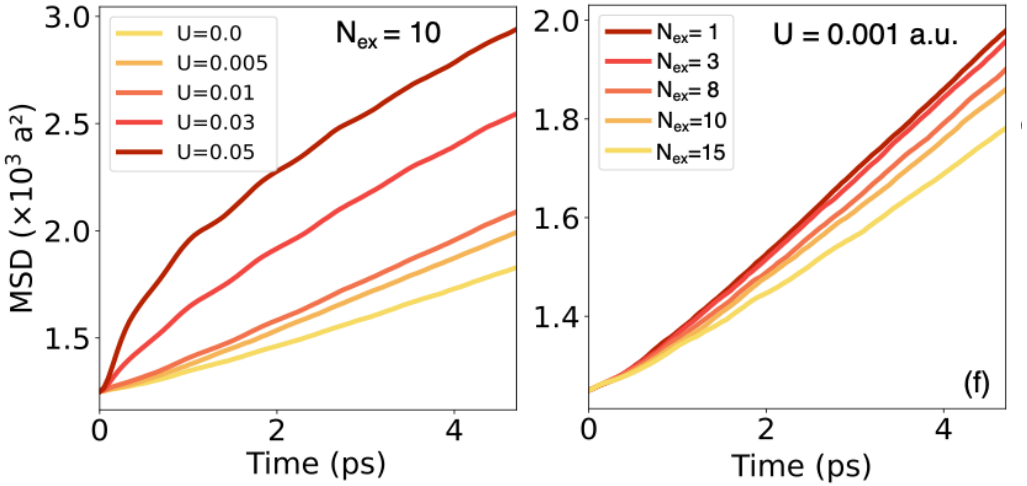
Quantum Dynamics of Bare Excitons



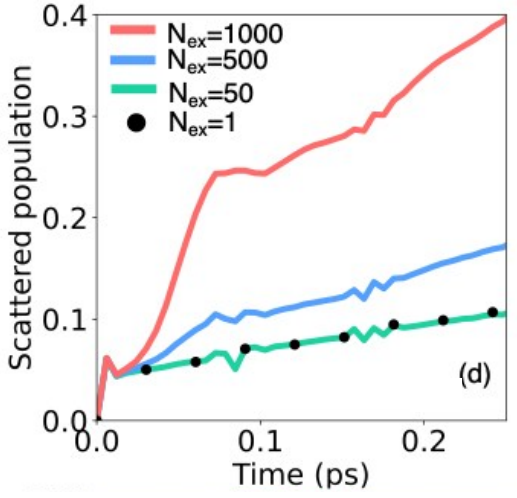
Quantum Dynamics of Exciton-polaritons (Non-interacting case)



Mean Square Displacement

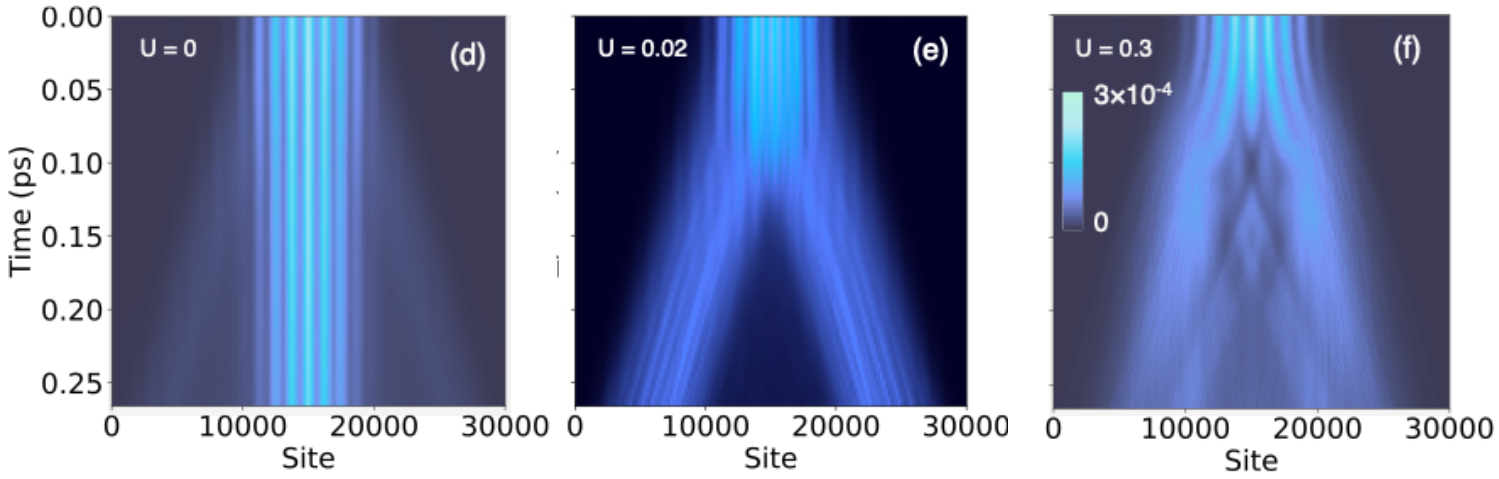


Dynamic Disorder Induced Scattering

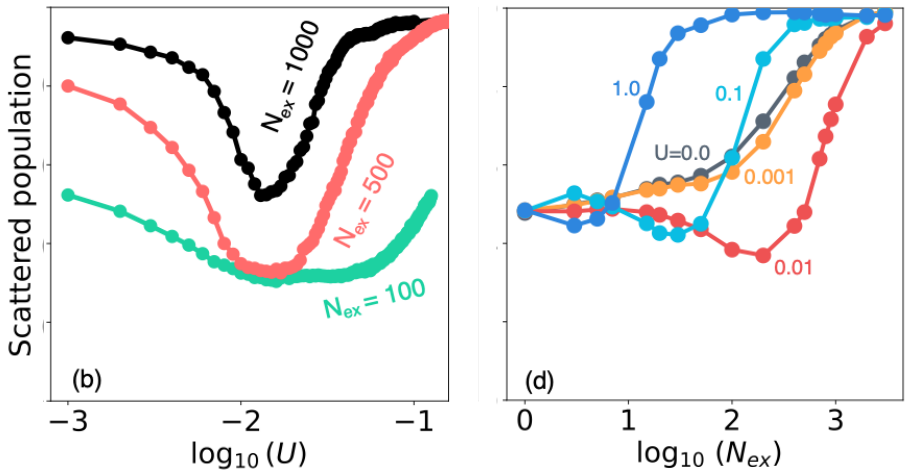


Results

Quantum Dynamics of Interacting Exciton-Polaritons



Interaction Strength Dependent Non-linearity



Many-body interactions can **combat** phonon induced decoherence.

Light & Matter Research Group at Texas A&M

Thank you

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