Theoretical description of BEC:
The Gross-Pitaevskii equation

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Derivation of Gross-Pitaevskii Equation

Bose-Einstein Condensate:
Gross-Pitaevskii Equation

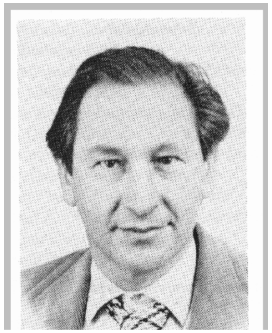
- Macroscopic numbers of particles is occupying the lowest energy level in the system
- All particles can be described by single wave-function, $\psi_0(\mathbf{r}, t)$ which is an order parameter of the system

Time-evolution of the condensate is described by the **Gross-Pitaevskii** equation

$$i\hbar\frac{\partial}{\partial t}\psi_0(\mathbf{r},t) = \left[-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r},t) + g|\psi_0(\mathbf{r},t)|^2\right]\psi_0(\mathbf{r},t)$$

Interaction coupling constant

Derivation of the Gross-Pitaevskii Equation (1961)



E. Gross

L. Pitaevskii

Heisenberg representation

$$i\hbar\frac{\partial}{\partial t}\widehat{\psi}(\mathbf{r},t) = [\widehat{\psi}(\mathbf{r},t),\widehat{H}]$$

field operator

$$\widehat{H} = \int \left(\frac{\hbar^2}{2m}\nabla\widehat{\psi}^\dagger\nabla\widehat{\psi}\right) d\mathbf{r} + \frac{1}{2}\int \widehat{\psi}^\dagger\widehat{\psi}^{\dagger\prime}V(r'-r)\widehat{\psi}\widehat{\psi}'d\mathbf{r}'d\mathbf{r}$$

Commutational relations:

$$[\widehat{\psi}(\mathbf{r}),\widehat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r}-\mathbf{r}')$$

$$[\widehat{\psi}(\mathbf{r}),\widehat{\psi}(\mathbf{r}')] = 0$$

$$i\hbar\frac{\partial}{\partial t}\widehat{\psi}(\mathbf{r},t) = \left[-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r},t) + \int \widehat{\psi}^\dagger(\mathbf{r}',t)V(\mathbf{r}'-\mathbf{r})\widehat{\psi}(\mathbf{r}',t)\right]\widehat{\psi}(\mathbf{r},t)$$

Derivation of the Gross-Pitaevskii Equation

$$i\hbar\frac{\partial}{\partial t}\widehat{\psi}(\mathbf{r},t) = \left[-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r},t) + \int \widehat{\psi}^\dagger(\mathbf{r}',t)V(\mathbf{r}'-\mathbf{r})\widehat{\psi}(\mathbf{r}',t)\right]\widehat{\psi}(\mathbf{r},t)$$

noncondensate component

$$\hat{\Psi}(\mathbf{r}) = \psi(\mathbf{r}) + \delta\hat{\Psi}(\mathbf{r})$$

condensate

$\widehat{\psi}(\mathbf{r},t)$ → $\psi_0(\mathbf{r},t)$

Realistic potential → Effective soft potential

By assuming that wave-function ***varies slowly*** on distances of the order of the range of the interatomic force, **r'** → **r**

$$i\hbar\frac{\partial}{\partial t}\psi_0(\mathbf{r},t) = \left[-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r},t) + g|\psi_0(\mathbf{r},t)|^2\right]\psi_0(\mathbf{r},t)$$

$$g = \int V_{eff}(\mathbf{r})d\mathbf{r} \longrightarrow g = \frac{4\pi\hbar^2 a}{m}$$

In the terms of scattering length a

The conditions of applicability of the GP equation

- The total number of atoms should be large, since only in this case we can use the concept of BEC.

- The physical properties of the gas are characterized by a scattering wave ***a*** and in
- particular, the condition of diluteness must be always satisfied.

$$|a| << n^{-1/3} \qquad\qquad n = \frac{N}{V} \quad \text{gas density}$$

- The temperature of gas is low enough.

- We are only allowed to investigate phenomena on a distances much larger than the scattering length. For microscopic lengths the approximations are no longer valid.

Bogoliubov-de Genne approximation

Some theoretical models describing BEC

Gross-Pitaevskii Equation (GPE)

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V_{\text{ext}}\psi + g|\psi|^2\psi$$

Complex Ginzburg-Landau Equation (CGLE)

$$i\mathrm{d}\phi = \left[A - B\frac{\partial^2}{\partial x^2} + C|\phi|^2 + i\left(D - E|\phi|^2\right)\right]\phi\,\mathrm{d}t$$

energy offset | disspersion coeff. | nonlinear interactions | pumping | nonlinear losses

Nonlinear Schrodinger equation (NLS)

$$i\frac{\partial\psi}{\partial t} + \frac{\partial^2\psi}{\partial x^2} - g|\psi|^2\psi = 0$$

Bogoliubov-de Gennes method (NLS)

$$i\frac{\partial \psi}{\partial t} + \frac{\partial^2 \psi}{\partial x^2} - g|\psi|^2\psi = 0$$

The elementary excitations spectrum around the stationary state of the system can be obtained by linearizing NLS around the steady-state solution.

$$\psi = \psi_0 e^{ipx - i\mu_0 t}\left[1 + \sum_k \{a_k e^{-i(\omega_k t - kx)} + b_k^* e^{i(\omega_k^* t - kx)}\}\right]$$

Eigenvalue problem

Theoretical models describing exciton-polariton BEC

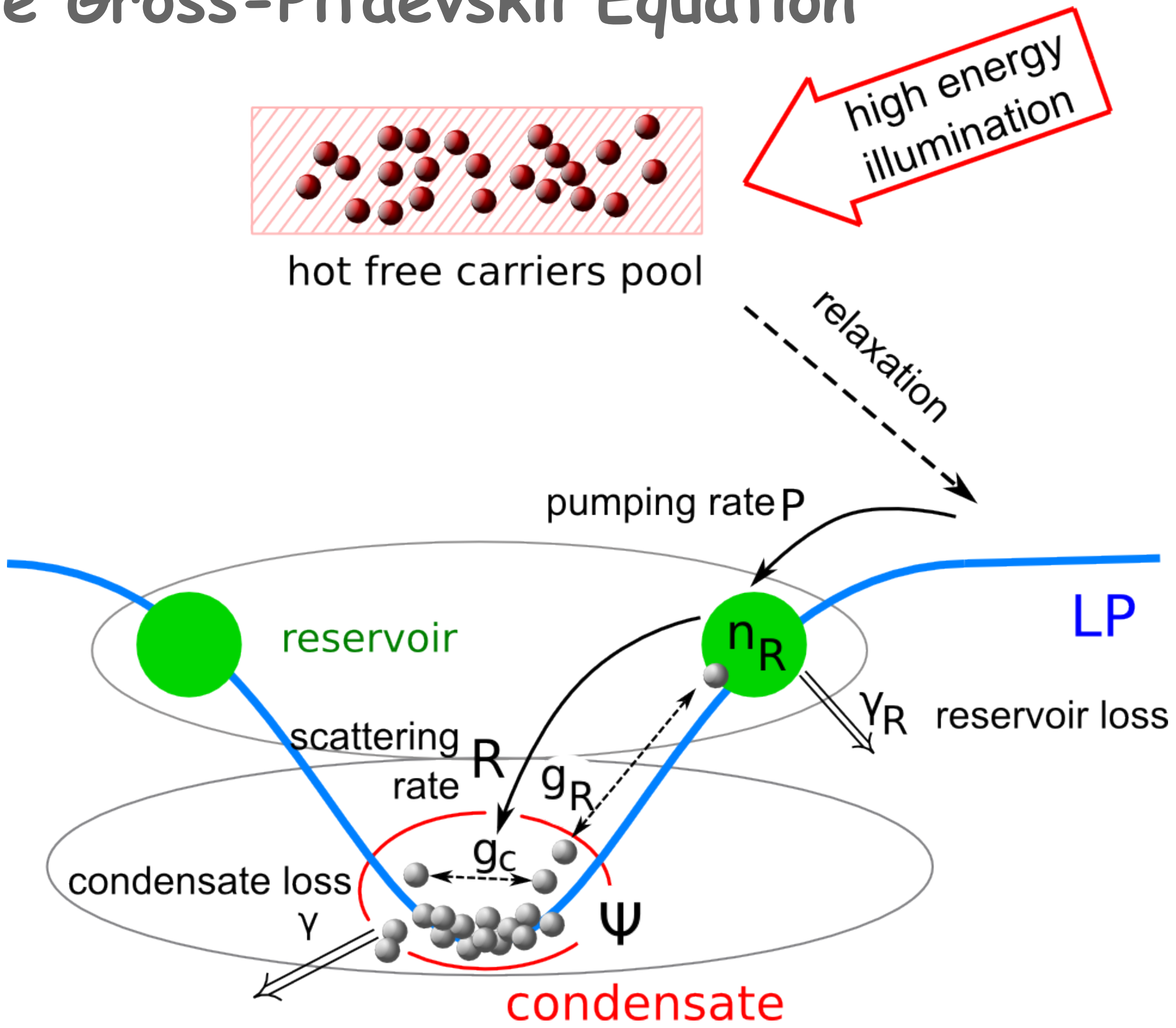
Gross-Pitaevskii Equation (GPE)

Complex Ginzburg-Landau Equation (CGLE)

Open-Dissipative Gross-Pitaevskii Equation (ODGPE)

Open-dissipative Gross-Pitaevskii Equation

Nonresonant excitation



Rate equation for the reservoir

$$\frac{\partial n_{\mathrm{R}}}{\partial t} = P(x) - (\gamma_{\mathrm{R}} + R^{1\mathrm{D}}|\psi|^2)n_{\mathrm{R}}$$

Gross-Pitaevskii equation describing condensate

$$i\hbar\frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2} + g_{\mathrm{C}}^{1\mathrm{D}}|\psi|^2 + g_{\mathrm{R}}^{1\mathrm{D}} n_{\mathrm{R}} + i\frac{\hbar}{2}\left(R^{1\mathrm{D}} n_{\mathrm{R}} - \gamma_{\mathrm{C}}\right)\right]\psi$$

Wouters and Carusotto, PRL 2007

Exciton-polariton condensation

Short lifetime
Strong interactions

→ **Constant pumping P**

to maintain system population
(balance between gain and loss)

Polariton condensation occurs when **P > P_th**

Homework: Calculation of threshold pumping, condensate and reservoir densities (1)

The **steady state** of the condensate under **homogeneous pumping** (**P(x) = P = *const***) can be obtained by substituting the ansatz

Complex constant

Note about notation:

$$\gamma_C = \gamma$$

$$g_C = g$$

$$\psi(x,t) = \psi_0 e^{-i\mu_0 t} \qquad (1)$$

$$n_R(x,t) = n_R^0 \qquad (2)$$

Real constant

into

here we switch to the dimensionless form of ODGPE

$$i\frac{\partial \psi}{\partial t} = \left[-\frac{\partial^2}{\partial x^2} + \frac{i}{2}\left(R n_R - \gamma\right) + g|\psi|^2 + g_R n_R\right]\psi \qquad (3)$$

$$\frac{\partial n_\mathrm{R}}{\partial t} = P(x) - (\gamma_\mathrm{R} + R|\psi|^2)n_\mathrm{R} \qquad (4)$$

Homework: Calculation of threshold pumping, condensate and reservoir densities (2)

HINTS:

1) **no condensate** is present for small values of P,

2) follow the idea: directly substitute ansatz into Eqs. (3) and (4),

3) something complex can be divided into Re and Im

Results

Below threshold pumping

$$\psi_0 = 0$$

$$n_R^0 = P/\gamma_R$$

NO CONDENSATE

Above threshold pumping

$$|\psi_0|^2 = (P/\gamma) - (\gamma_R/R)$$

$$n_R^0 = \gamma/R$$

$$\mu_0 = g|\psi_0|^2 + g_R n_R^0$$

CONDENSATE

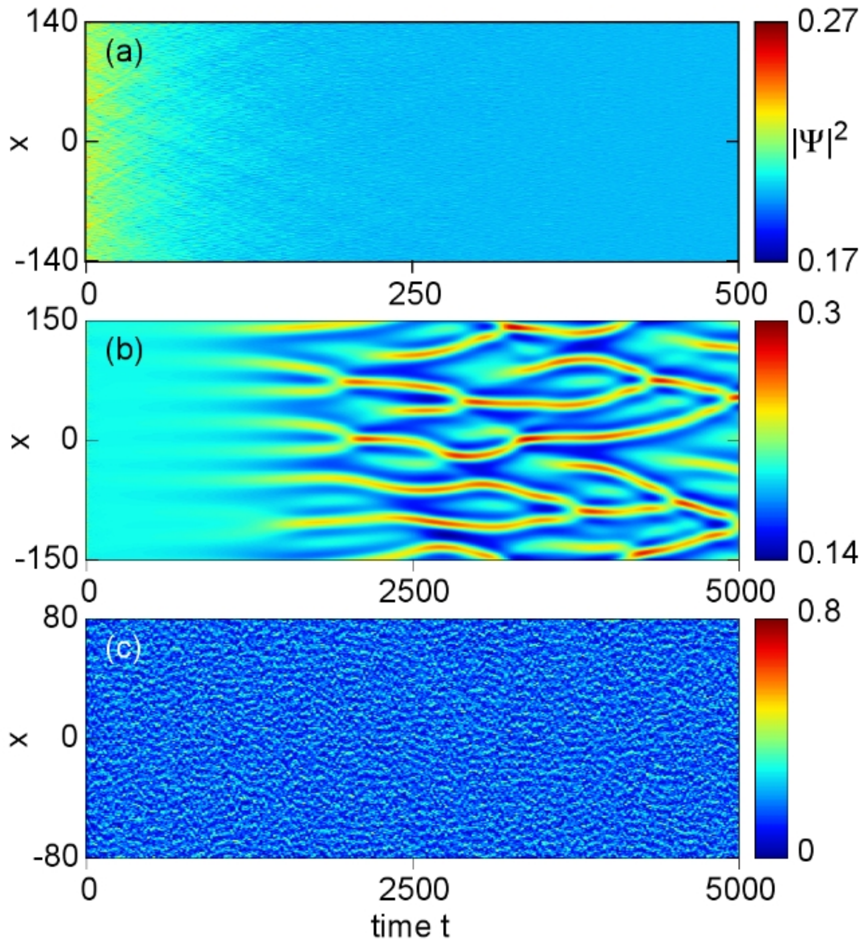
Threshold pumping

$$P_{th} = \gamma\gamma_R/R$$

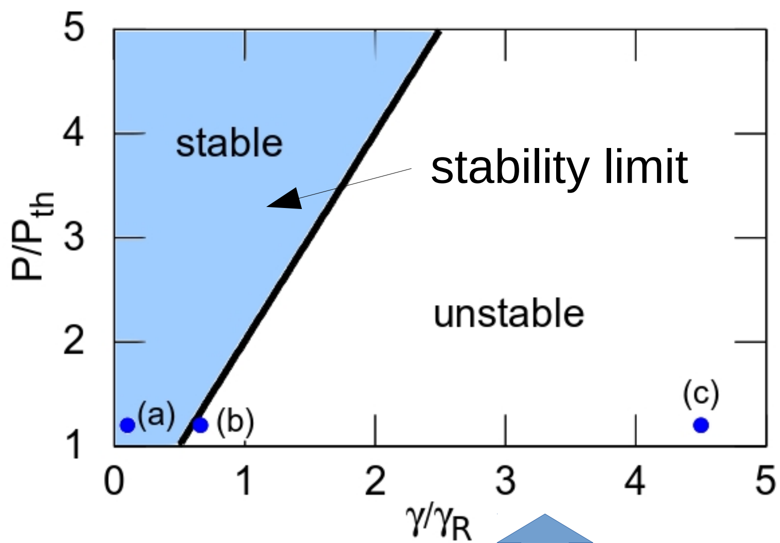
Condensate stability

Homogeneous pumping – stability diagram

Density evolution of the condensate



Stability diagram



The analytical condition
for condensate stability

$$\frac{P}{P_{th}} > \frac{g_R}{g} \frac{\gamma}{\gamma_R}$$

Periodic boundary conditions

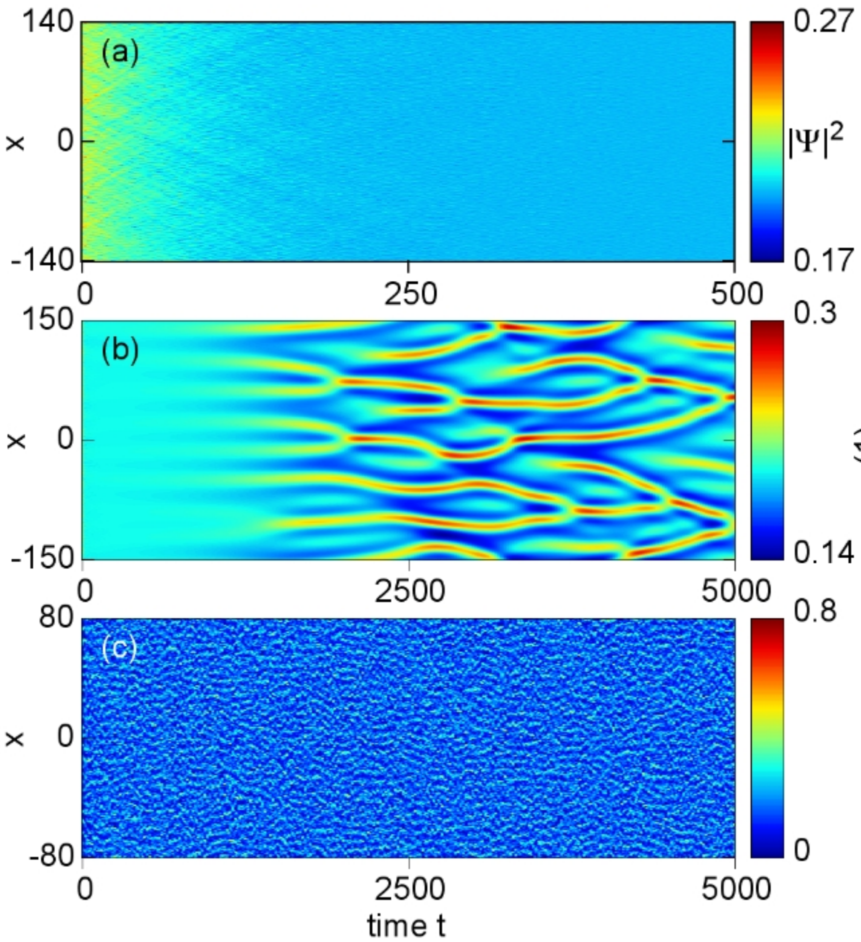
(stability diagram
could be obtained analytically)

Bobrovska et al., PRB 2014

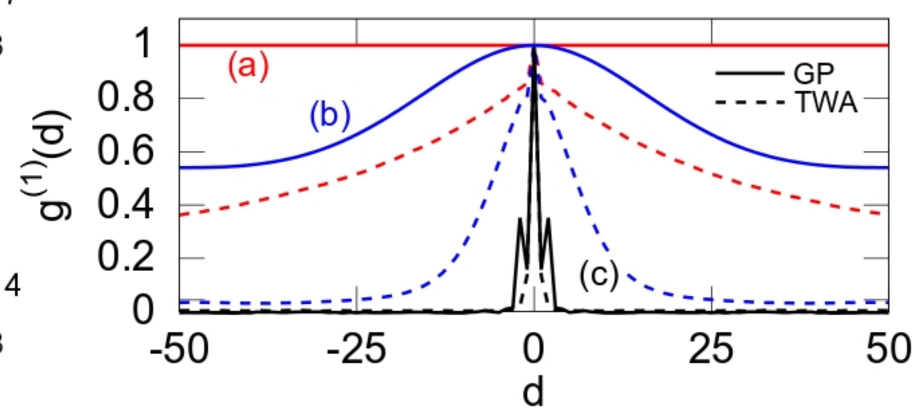
Smirnov et al., PRB 2014

Homogeneous pumping – correlation function

Density evolution of the condensate



First-order correlation function



$$g^{(1)}(d) = \langle \psi^*(x)\psi(x+d)\rangle / \langle |\psi(x)|^2 \rangle$$

Homogeneous pumping – Energy relaxation

The equation for the condensate wavefunction in ODGPE model
is extended by adding the relaxation term

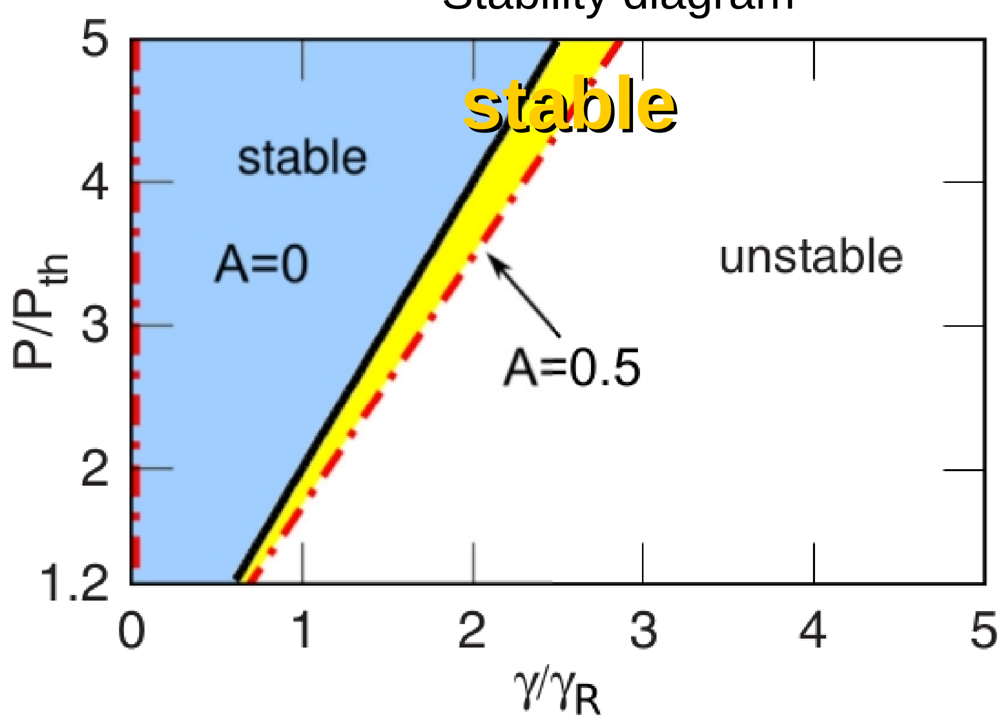
$$\frac{\partial \psi}{\partial t} = \left[(i + A) \frac{\partial^2}{\partial x^2} + \frac{1}{2}(R n_R - \gamma) - i g |\psi|^2 - i g_R n_R \right] \psi$$

$$\frac{\partial n_{\mathrm{R}}}{\partial t} = P(x) - (\gamma_{\mathrm{R}} + R|\psi|^2) n_{\mathrm{R}}$$

relaxation term

Tanese et al, Nat. Commun. 2013

Stability diagram



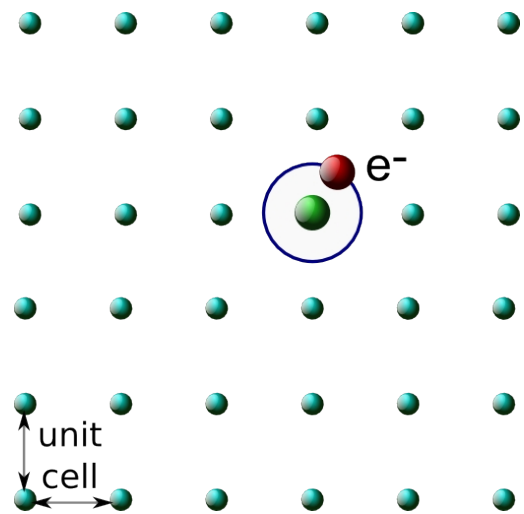
(Stability diagram
could be obtained analytically)

Such modification of ODGPE system has small effect on the condensate stability

Organic and inorganic exciton-polariton condensates

Exciton classification

- single lattice site,molecule
- Bohr rad.
  ~few of angstroms
- Perturbation:
  crystal potential
  with respect to
  Coulomb interactions
- Large binding energy
  ~100-300 meV



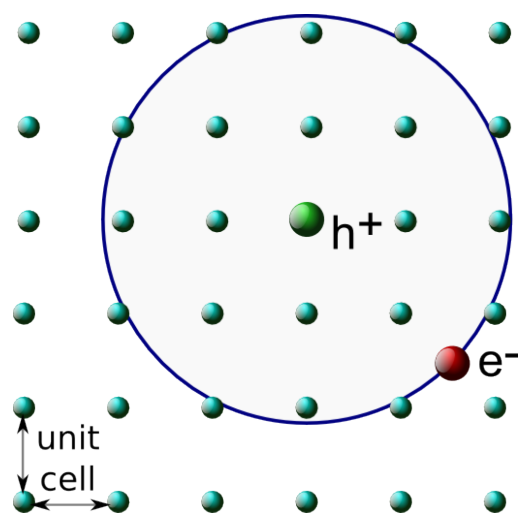
Y. I. Frenkel
(1894–1952)

Frenkel exciton

Organic semiconductors

?

- many lattice sites
- Bohr rad.~tens to
  hundreds of angstroms
- Perturbation: Coulomb
  attraction with
  respect to
  crystal potential
- Small binding energy
  ~ few-tens meV



N. F. Mott
(1905–1996)

G. Wannier
(1911–1983)

Inorganic semiconductors

Wannier-Mott exciton

Exciton classification

- single lattice site,molecule
- Bohr rad.
  ~few of angstroms
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  crystal potential
  with respect to
  Coulomb interactions
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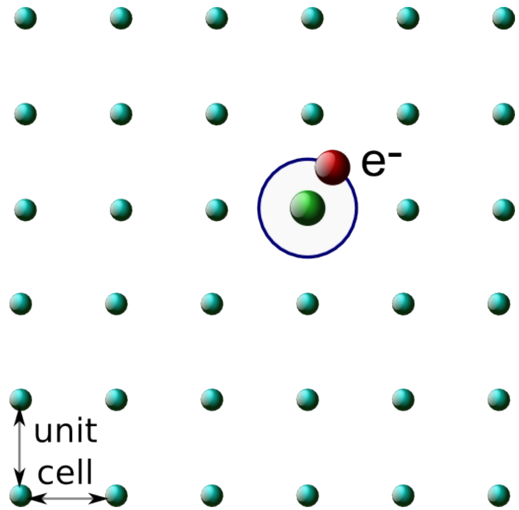


Y. I. Frenkel
(1894–1952)

Frenkel exciton

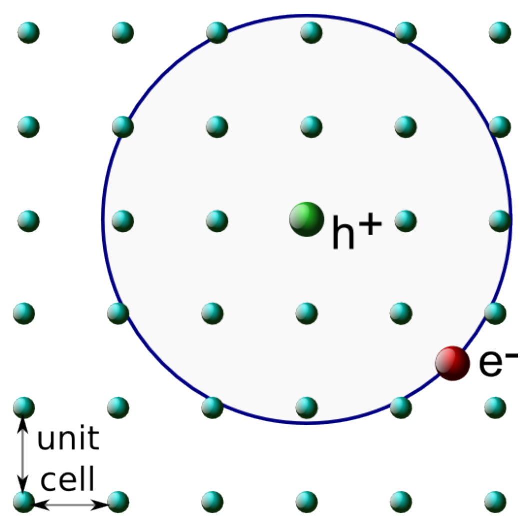
Organic semiconductors

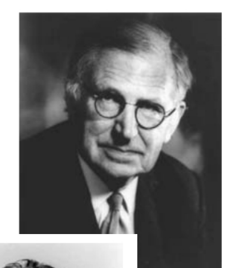
charge–transfer excitons, anyon exciton

hybrid Frenkel–Wannier–Mott excitons

mixed organic–inorganic structures

- many lattice sites
- Bohr rad.~tens to
  hundreds of angstroms
- Perturbation: Coulomb
  attraction with
  respect to
  crystal potential
- Small binding energy
  ~ few-tens meV





N. F. Mott
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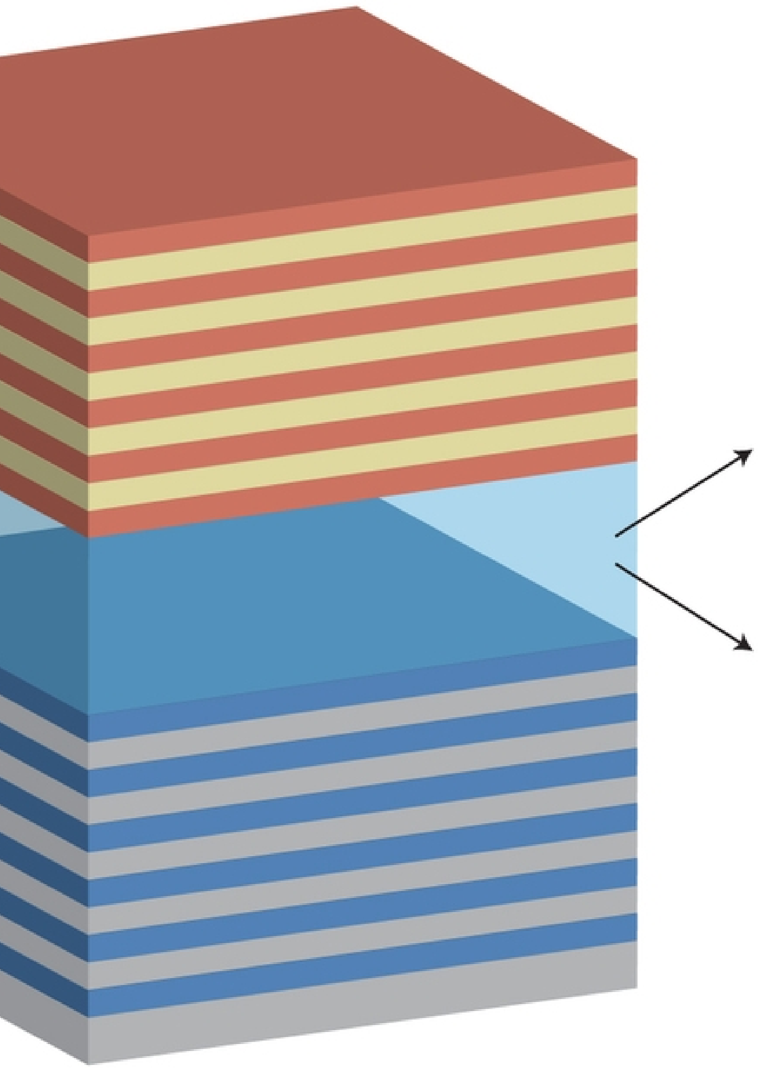
Inorganic semiconductors

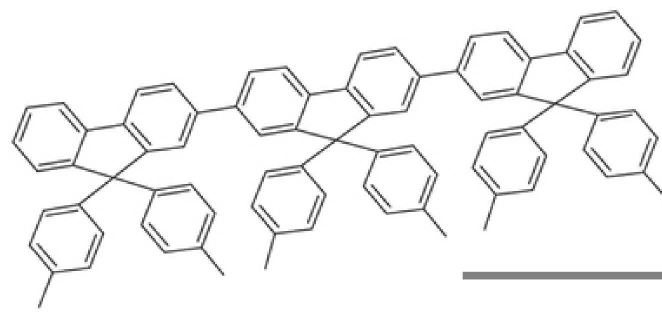
Wannier-Mott exciton

“Going soft” - organic optical microcavities



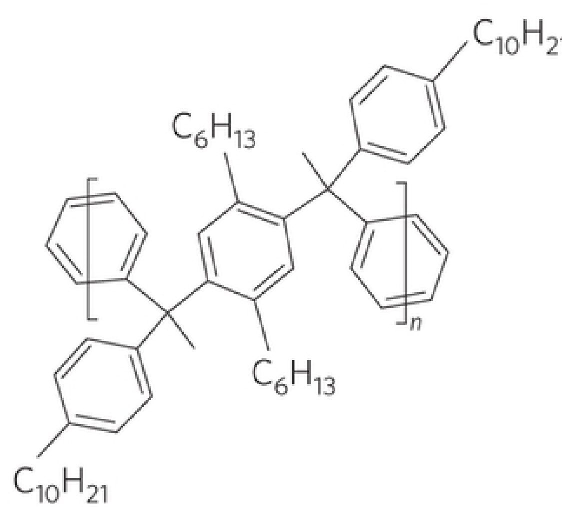
oligofluorene (TDAF)

2,7-bis[9,9-di(4-methylphenyl)-fluoren-2-yl]-9,9-di(4-methylphenyl)fluorene



group of
Stefane Kena-Cohen*

MeLPPP polymer



methyl-substituted
ladder-type poly(p-phenylene)

group of
Rainer F. Mahrt**

Lagoudakis, Nature Mater. 2014

***Johannes et al, Nature Mater. 2014*
**Daskalakis et al, Nature Mater. 2014*

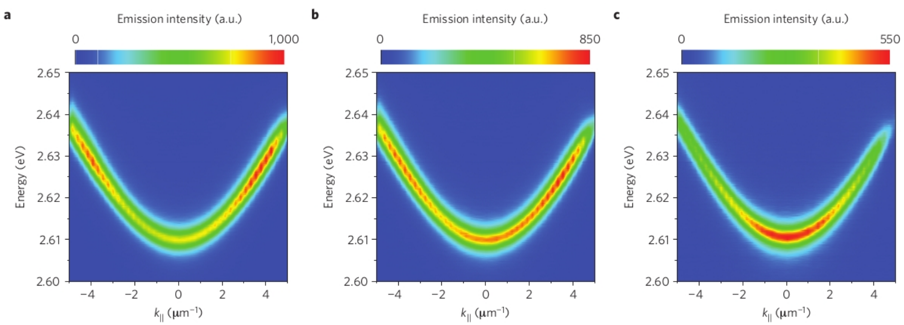
Examples of organic exciton-polariton condensates

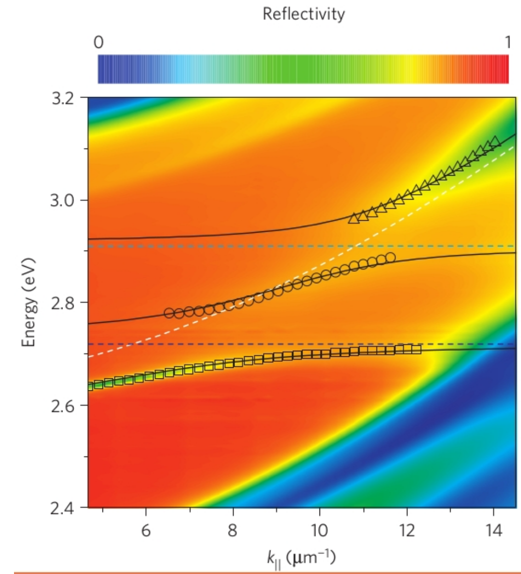
nature materials | LETTERS

PUBLISHED ONLINE: 8 DECEMBER 2013 | DOI:10.1038/NMAT3825

Room-temperature Bose–Einstein condensation of cavity exciton–polaritons in a polymer

Johannes D. Plumhof[1†], Thilo Stöferle[1*], Lijian Mai[1], Ullrich Scherf[2] and Rainer F. Mahrt[1]





--- exciton

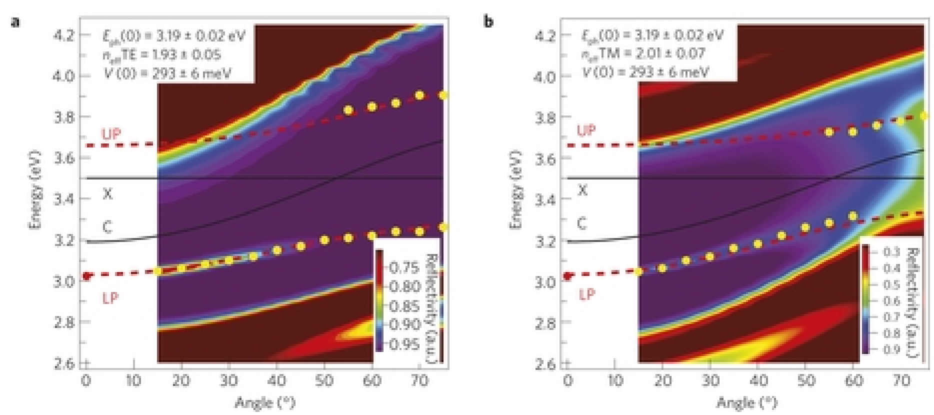
--- photon

Nonlinear interactions in an organic polariton condensate

K. S. Daskalakis, S. A. Maier, R. Murray & S. Kéna-Cohen

Affiliations | Contributions | Corresponding author

Nature Materials **13**, 271–278 (2014) | doi:10.1038/nmat3874



transverse electric (TE) transverse magnetic(TM)
polarizations

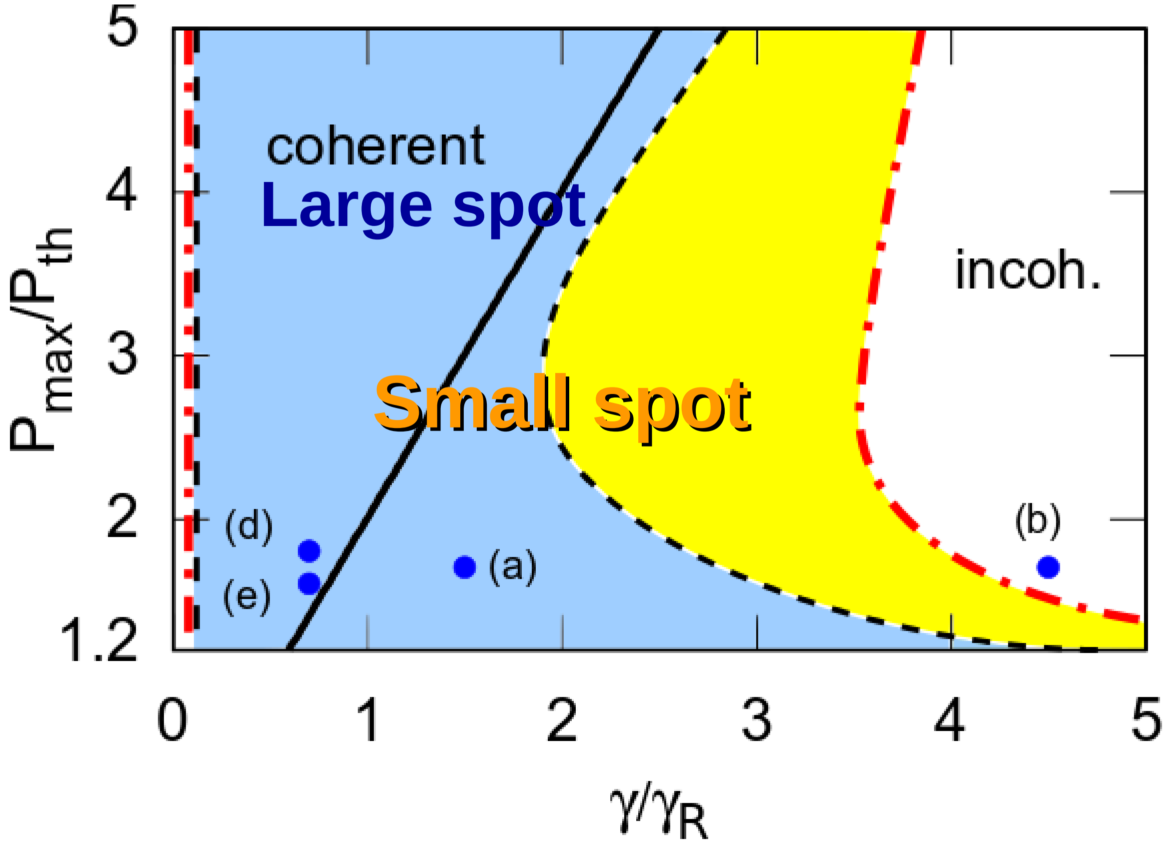
Systems are excited by incoherent off-resonant optical pumping (ps pulses)

Inhomogeneous pumping

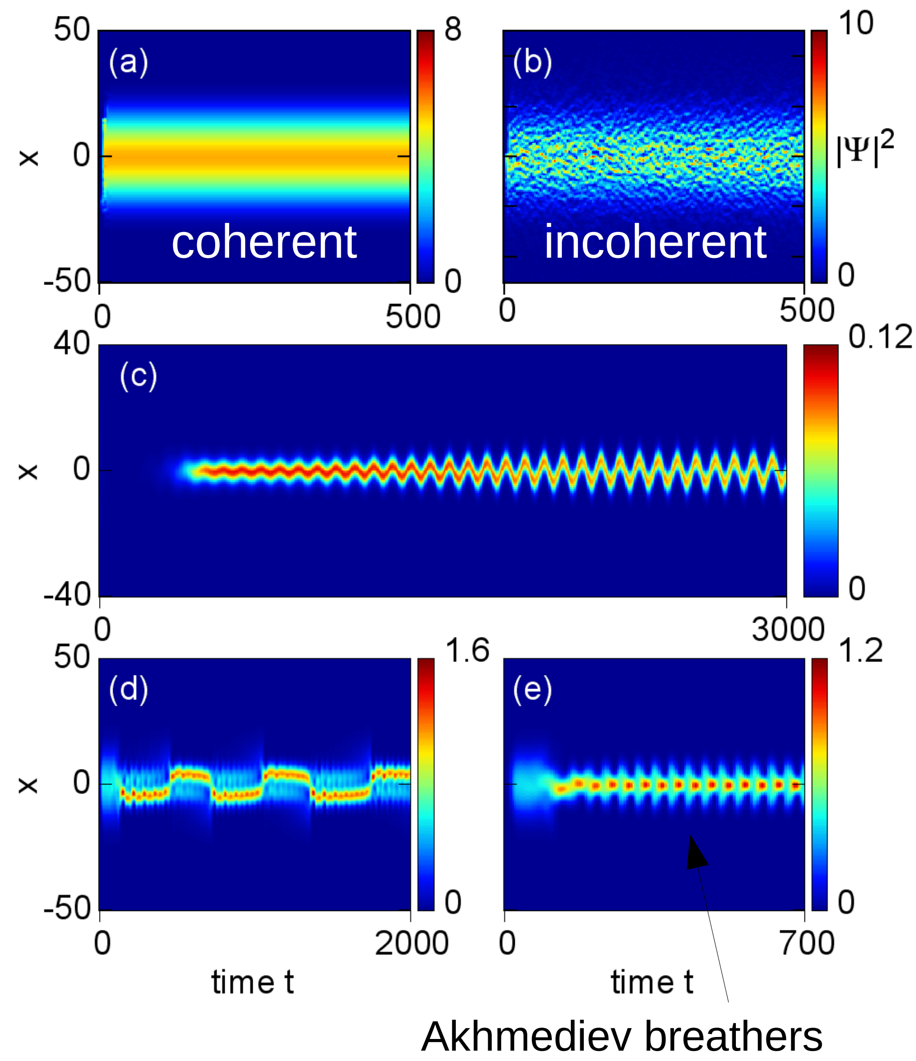
Gaussian profile

$$P(x) = P_{\max} \exp(-x^2/W^2).$$

(stability diagram could be obtained only numerically



Density evolution of the condensate



In the case of inhomogeneous pumping condensate is coherent or incoherent
(stable or unstable in the case of ho,ogeneous pumping, P=const)

Stability of polariton condensates - conclusions

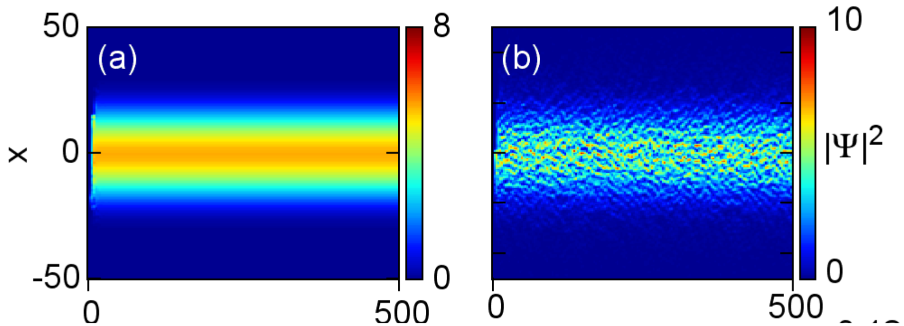
Homogeneous pumping

- Instability in steady state leads to a significant reduction of the condensate coherence
- The polariton energy relaxation has a little effect on the condensate stability

Inhomogeneous pumping

- Pumping profile has significant effect on the condensate stability and changes the condensate coherence length

1D



2D