A rigorous computational framework employing coupled-mode theory for assessing lasing with transition metal dichalcogenide bilayers in the nanoscale

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I Introduction

Motivation

- **Transition metal dichalcogenide (TMD) hetero-bilayers** constitute the most promising family of **2D gain materials**.
- Incorporation of TMD hetero-bilayers in **micro-** and **nano-cavities** for low lasing threshold and compact-sized **light sources in the near infrared (NIR)**.

Objectives

- Develop a rigorous and flexible framework based on **temporal coupled-mode theory (CMT)** and **perturbation theory** to describe both bulk and sheet gain media.
- Exploit the framework to design a **MoS_2/WSe_2**-enhanced silicon-rich-nitride-on-insulator (SRNOI) whispering-gallery mode (**WGM**) **disk resonator laser**.

II CMT framework for 2D gain materials

- General and robust framework of **first-order** nonlinear ordinary differential equations (**ODEs**) derived rigorously by **Maxwell-Bloch equations** [1].

1. **Stimulated transition** is treated through a **surface polarization field.**

$$\nabla \times \boldsymbol{\mathcal{E}}(\mathbf{r},t) = -\mu_0 \frac{\partial \boldsymbol{\mathcal{H}}(\mathbf{r},t)}{\partial t}$$

$$\nabla \times \boldsymbol{\mathcal{H}}(\mathbf{r},t) = \varepsilon_0 \varepsilon_\mathrm{r} \frac{\partial \boldsymbol{\mathcal{E}}(\mathbf{r},t)}{\partial t} + \boxed{\frac{\partial \boldsymbol{\mathcal{P}}_{||}(\mathbf{r},t)}{\partial t}\delta_S(\mathbf{r})}$$

2. Utilizing first-order **perturbation theory** [2] and the **Lorentz reciprocity theorem** [3], the **complex resonance frequency shift** induced by the polarization field is evaluated.

$$\Delta\tilde{\omega}(t) = j\xi_1 \frac{1}{a(t)}\left[j\omega_\mathrm{c} p(t) + \frac{\mathrm{d}p(t)}{\mathrm{d}t}\right] \qquad \boxed{\xi_1 = \frac{1}{4}\iint_{S_g} |\mathbf{E}_{\mathrm{ref},||}|^2 \mathrm{d}S}$$

3. The **cavity amplitude equation** is derived, and the feeding parameters are calculated through **Finite Element Method (FEM)** simulations.

$$\frac{\mathrm{d}a(t)}{\mathrm{d}t} = -j(\omega_\mathrm{ref} - \omega_\mathrm{c})a(t) - \frac{1}{\tau_\ell}a(t) + j\Delta\tilde{\omega}(t)a(t)$$

4. The surface polarization field follows the equation of a **homogeneously broadened Lorentzian transition** [1].

$$\frac{\partial^2 \boldsymbol{\mathcal{P}}_{||}(\mathbf{r},t)}{\partial t^2} + \Gamma_m \frac{\partial \boldsymbol{\mathcal{P}}_{||}(\mathbf{r},t)}{\partial t} + \omega_m^2 \boldsymbol{\mathcal{P}}_{||}(\mathbf{r},t) = -\sigma_m \Delta N_s(\mathbf{r},t)\boldsymbol{\mathcal{E}}_{||}(\mathbf{r},t)$$

5. It is introduced in the CMT framework by exploiting the **slowly-varying envelope approximation (SVEA)**.

$$\frac{\mathrm{d}p(t)}{\mathrm{d}t} = -\frac{\omega_m^2 - \omega_\mathrm{ref}^2 + j\omega_\mathrm{ref}\Gamma_m}{\Gamma_m + j2\omega_\mathrm{ref}}p(t) - \frac{\sigma_m}{\Gamma_m + j2\omega_\mathrm{ref}}\Delta\bar{N}_s(t)a(t)$$

6. The carrier dynamics are described by semiclassical **carrier rate equations.**

$$\frac{\mathrm{d}\bar{N}_{2,s}(t)}{\mathrm{d}t} = \frac{\xi_2}{2\hbar\omega_m}\mathrm{Re}\left\{\left[j\omega_\mathrm{ref}p(t) + \frac{\mathrm{d}p(t)}{\mathrm{d}t}\right]a^*(t)\right\} - \frac{\bar{N}_{2,s}(t)}{\tau_{21}} + \frac{\bar{N}_{3,s}(t)}{\tau_{32}}$$

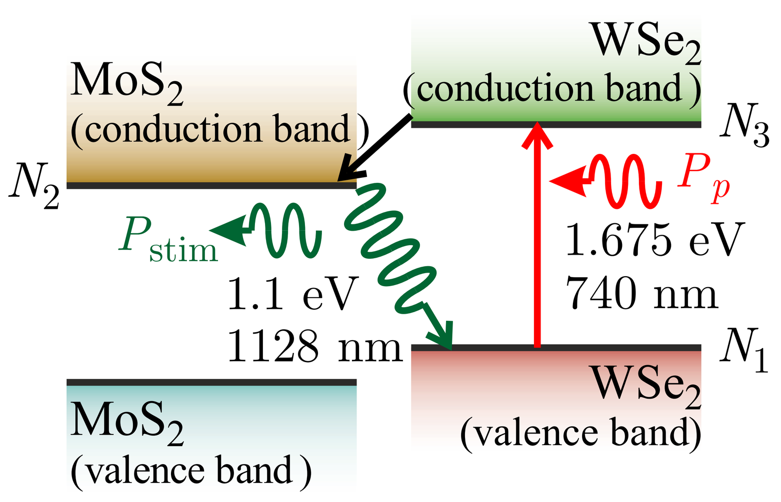
- For a **three-level** gain medium the framework consists of **five** first-order **ODEs** (cavity amplitude, polarization and three carrier rate equations).

$$\boxed{\xi_2 = \frac{\iint_{S_g} |\mathbf{E}_{\mathrm{ref},||}|^4 \mathrm{d}S}{\iint_{S_g} |\mathbf{E}_{\mathrm{ref},||}|^2 \mathrm{d}S}}$$

III The MoS_2/WSe_2 TMD hetero-bilayer

- **Three-level** gain medium.
- Gain provided by the radiative recombination of **interlayer excitons** [4].

τ_{32} = 100 fs	λ_m = 1128 nm
τ_{21} = 1 ns	λ_p = 740 nm
Γ_m = 20 Trad/s	$\bar{N}_\mathrm{tot}$ = 10^{13} cm^{-2}



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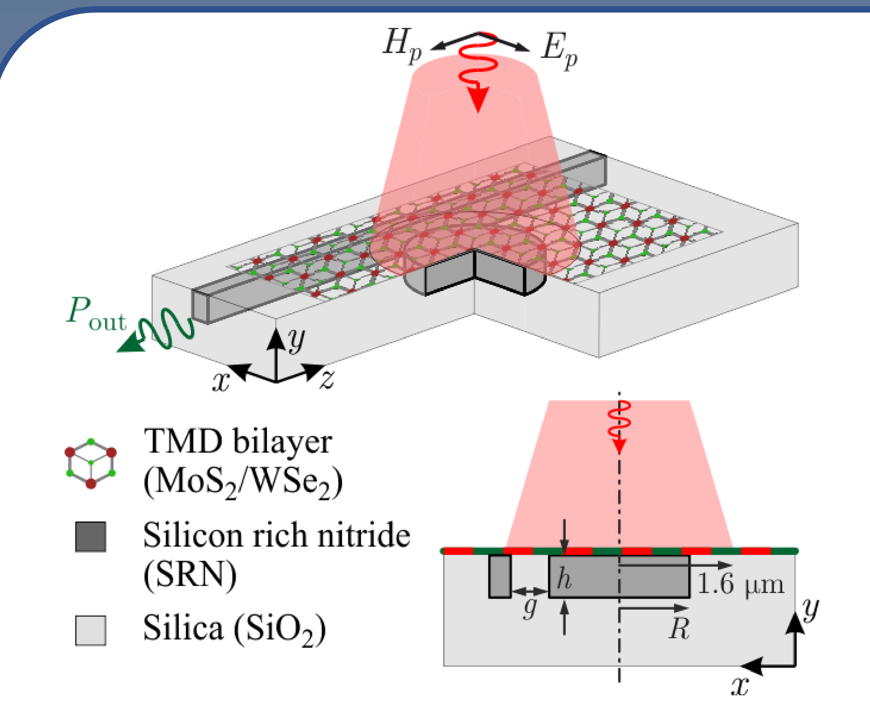
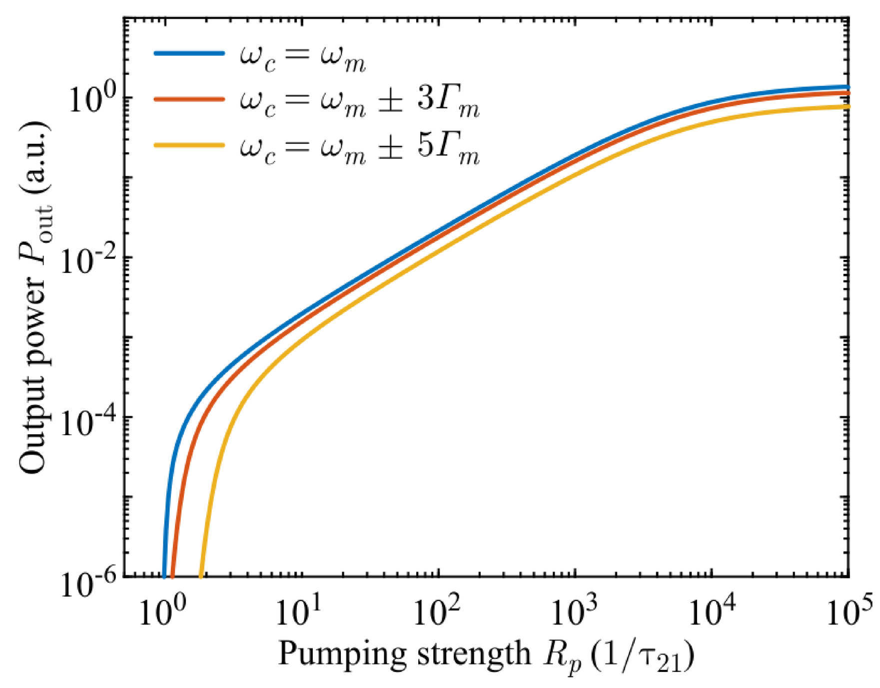
IV Laser structure

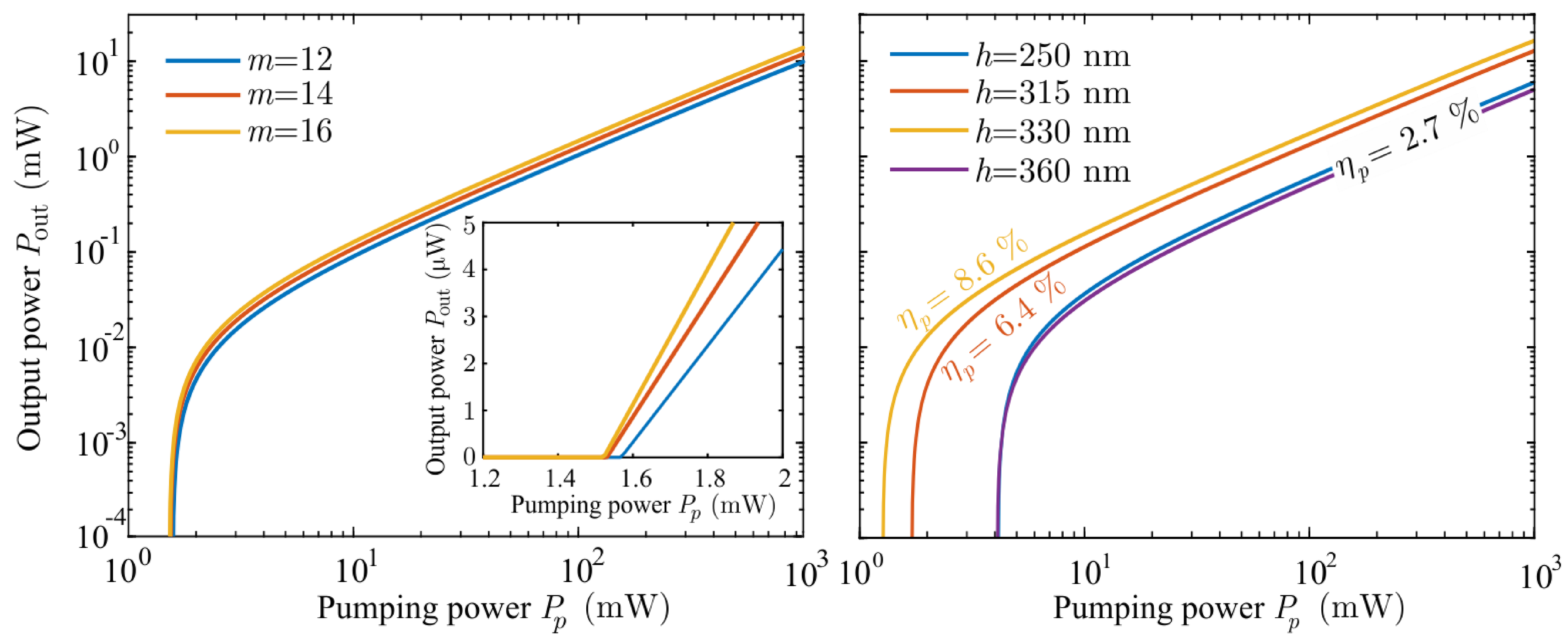


- SRNOI disk resonator supporting WGMs with **high Q-factors**.
- MoS_2/WSe_2 on top of the disk resonator to **maximize light-matter interaction**.
- **Bus waveguide** side-coupled to the cavity to extract the emitted light.
- **Optical pump** with free-space beam.
- SRN is **transparent** at both the emission and pumping wavelengths.

Cavity Design



- The lasing **threshold** is **minimized** and the **output power maximized** for $\boldsymbol{\omega_m = \omega_c}$.
- In the general case that $\omega_m \neq \omega_c$, the **lasing frequency ω_L** does not coincide with ω_m or ω_c; nevertheless, it can be **accurately estimated** by the developed CMT framework.



- Greater **WGM mode order** (greater **radius *R*** of the disk resonator) results in improvement of both lasing threshold and output power.
- The **height of the resonator** affects the **absorption efficiency** of the pumping power, η_p, due to the formation of a **vertical Fabry-Pérot cavity** when the structure is pumped. **η_p maximizes for h = 330 nm** leading to lowest lasing threshold and maximum output power.

$P_{p,\mathrm{th}}$ = 1.3 mW			R = 1.317 μm	
$\Delta\bar{N}_\mathrm{th}$ = 4.61x10^{10} cm^{-2}			h = 330 nm	
			g = 300 nm	
Q_i = 101 500	Q_e = 9600	η_p = 8.6 %	ξ_1 = 8.93x10^{15} V/C	ξ_2 = 1.29x10^{28} V/(Cm^2)

V Conclusion

A **rigorous framework** based on temporal **CMT** and perturbation theory has been presented capable of treating contemporary **2D gain materials** and accurately evaluating **fundamental lasing characteristics** of micro/nano-cavity lasers. Utilizing the framework, a **practical laser element** consisting of a SRNOI disk resonator with the gain provided by a **MoS_2/WSe_2** hetero-bilayer has been designed, exhibiting **low lasing threshold** at a pump of **1.3 mW**.

VI References

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