Polaritonic features in the THz displacement current through RTDs in microcavities

Carlos F. Destefani *, Matteo Villani *, Xavier Cartoixà *, Michael Feiginov **, Xavier Oriols *

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(electrons and fields at the same foot)

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INTRO

Matter (electrons)

- Micrometer or larger sizes

Semiclassical models. Electrons as particles. Trajectories, …

- Nanometer scale

Quantum models. Energy level quantization. NDR, …

Electromagnetic fields

- GigaHertz or smaller frequencies

Poisson equation ($\boldsymbol{E}_{\parallel}(\boldsymbol{r})$) within a quasistatic approximation.

- 0.1-10 TeraHertz (THz gap)

Maxwell equations ($\boldsymbol{E}_{\perp}(\boldsymbol{r}),\boldsymbol{B}_{\perp}(\boldsymbol{r})$) coupled to a transport model.

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Nanoscale devices at THz (RTDs in enginnered microcavities)

- Similar energy scales. Quantization of both electrons and electromagnetic fields.
- Light-matter resonant coupling parameter $\gamma = \omega_r/\omega$ [$\omega = (E_1 - E_0)/\hbar$, ω_r = Rabi].
- Closed system models: Jaynes-Cummings, ...
- Open system models: ???

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Small coupling ($\gamma < 0.1$)

- Perturbative models. Fermi Golden Rule.
- Collisions. Photon absorption/emission.

- Experimental advances.
- Platforms with $\gamma = 1.2$.

Strong coupling ($\gamma > 0.5$)

- Need of new theoretical models.
- 3N-electron 2M-mode undoable. QEDFT, …

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- Effective single-electron ballistic picture.
- Resonant single-mode cavity field.
- Dipole approximation ($\lambda_{cavity} \gg W_{device}$).

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Our work

- Qualitative initial model for nanoscale at THz within strong coupling.
- Born-Huang wavefunction. Ramo-Shockley-Pellegrini current.
- Signatures of field quantization in electron transport are identifiable?

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Resonant tunneling diodes strongly coupled to the cavity field

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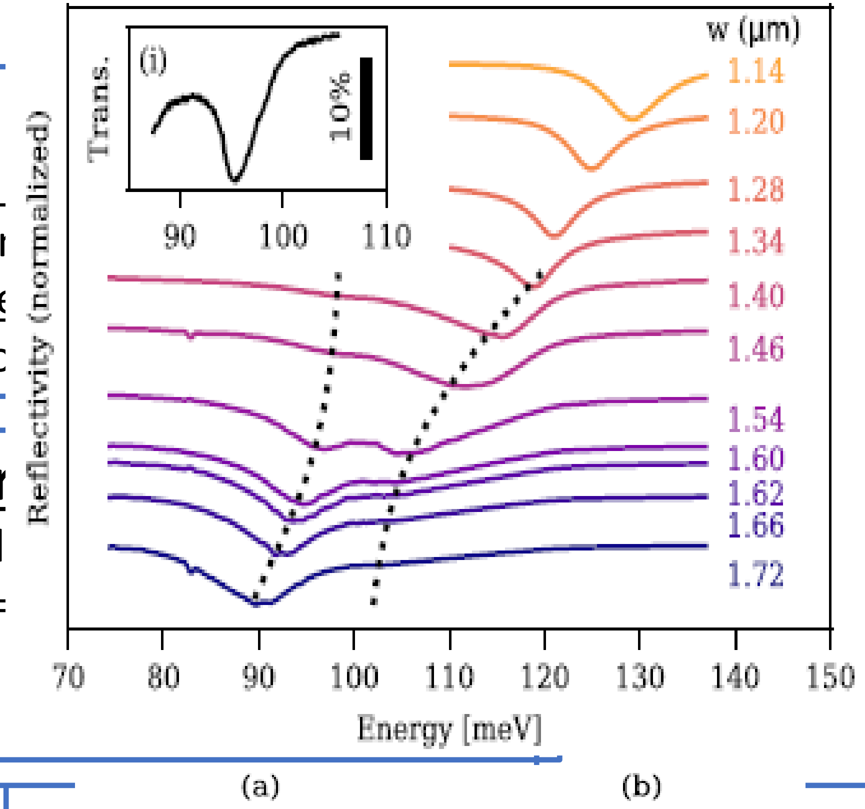

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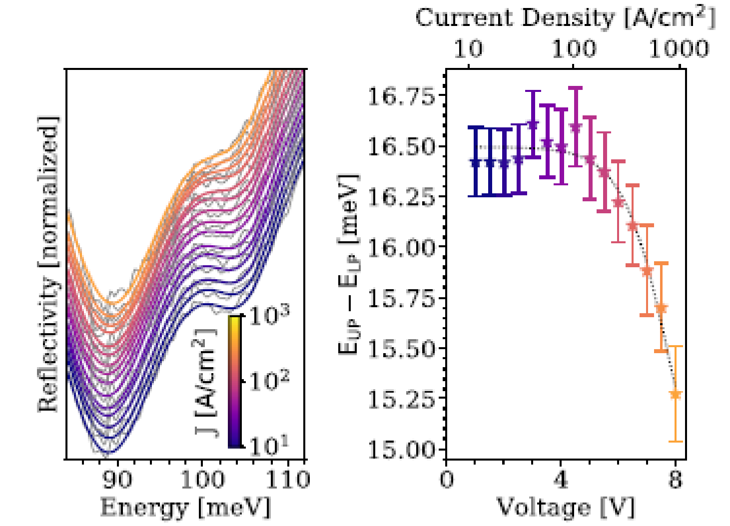
DFT, ...



Realistic approximations

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HAMILTONIAN ($H = H_0 + H_{\omega 0}$)

Spinless non-relativistic minimal coupling (Coulomb gauge, dipole approximation)

$$H_0 = \sum_{j=1}^{N} \left\{ \frac{1}{2m_e} [i\hbar\nabla_j + e\mathbf{A}(\mathbf{r}_j)]^2 + eU(\mathbf{r}_j) + V(\mathbf{r}_j) \right\}$$

Longitudinal field $\boldsymbol{E}_{\parallel}(\boldsymbol{r})$

Transversal fields

$$H_{\omega 0} = \frac{\epsilon_0}{2} \int d^3\mathbf{r} [\mathbf{E}_{\perp}^2(\mathbf{r}) + c^2 \mathbf{B}_{\perp}^2(\mathbf{r})]$$

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Quantization procedure ($n = 1, \ldots, M$; $\lambda = 1,2$)

$\boldsymbol{E}_{\perp}(\boldsymbol{r}), \boldsymbol{B}_{\perp}(\boldsymbol{r})$ in terms of vector potential. $\boldsymbol{A}(\boldsymbol{r})$ in terms of creation/anihillation operators.

$a_{n,\lambda}^{\dagger}/a_{n,\lambda}$ in terms of displacement coordinates $q_{n,\lambda}$and their conjugate momenta $\partial/\partial q_{n,\lambda}$.

$$a_{n,\lambda} = \frac{1}{\sqrt{2}} \left(q_{n,\lambda} + \frac{\partial}{\partial q_{n,\lambda}} \right)$$

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Power-Zienau-Wooley (PZW) gauge transformation (3N + 2M degrees)

$$\{ \chi_{n,\lambda} = i/\sqrt{2\epsilon_0\hbar\omega_n L_c^3}\epsilon_{n,\lambda} \cdot e\sum_{j=1}^{N}\mathbf{r}_j \}$$

$$H^{(D)} = \underbrace{\sum_{j=1}^{N}\left[-\frac{\hbar^2\nabla_j^2}{2m_e} + V(\mathbf{r}_j) + eU(\mathbf{r}_j)\right]}_{H_e^{(D)}} + \underbrace{\sum_{n,\lambda}\hbar\omega_n|\chi_{n,\lambda}|^2}_{\varepsilon_{s-dip}} + \sum_{n,\lambda}\left(\underbrace{\frac{\hbar\omega_n}{2}\left[q_{n,\lambda}^2 - \frac{\partial^2}{\partial q_{n,\lambda}^2}\right]}_{H_f^{(D)}} + \underbrace{\sqrt{2}\hbar\omega_n|\chi_{n,\lambda}|q_{n,\lambda}}_{H_{ef}^{(D)}}\right)$$

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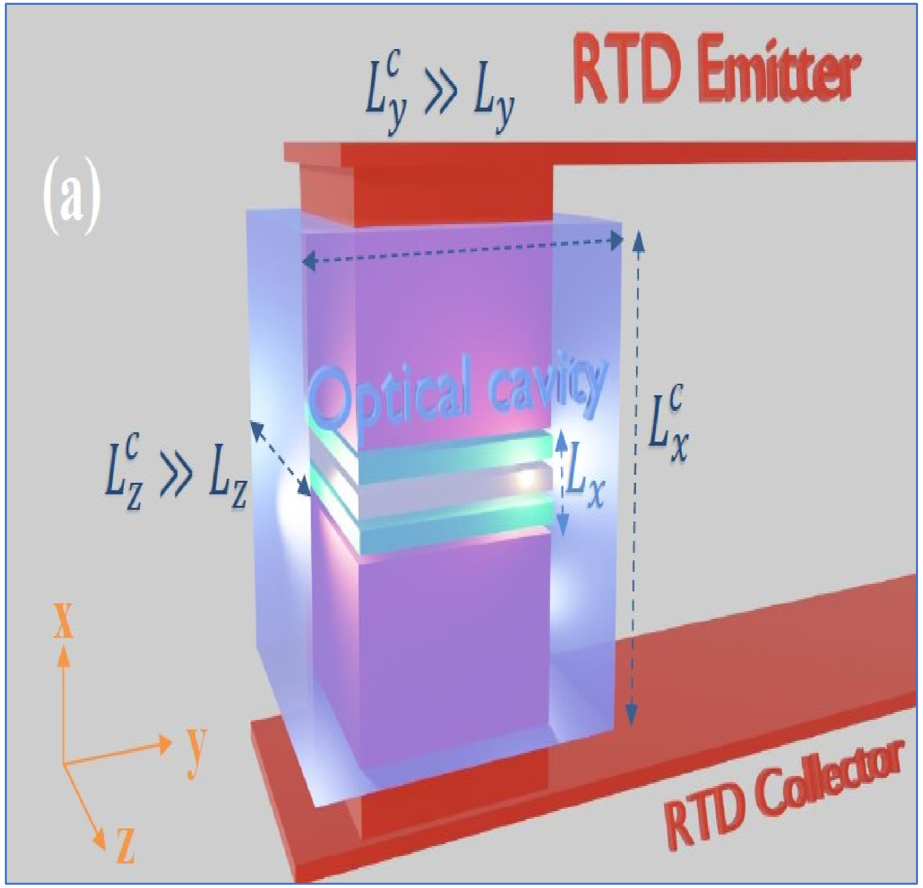
Initial approximations and use of conditional wave functions (effective 2D problem: single electron *x*, single mode *q*)

$$H_{xq}^{(D)} = -\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial x^2} + V(x) - \frac{\hbar\omega}{2}\frac{\partial^2}{\partial q^2} + \frac{\hbar\omega}{2}q^2 + \sqrt{2}\alpha q x$$

$$\alpha = \sqrt{e^2\hbar\omega N/(2\epsilon_0 L_c^3)}$$

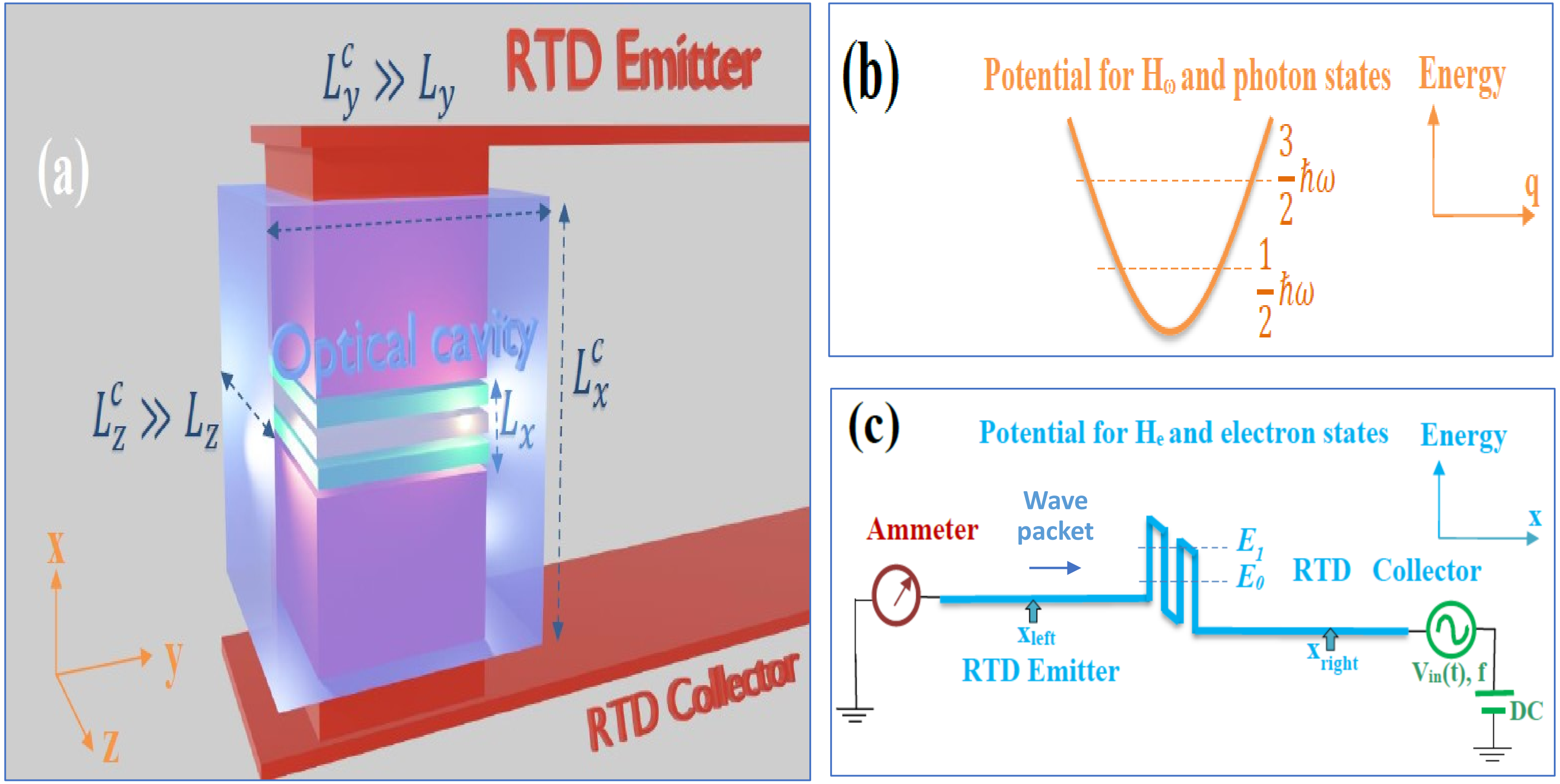
$$\omega_r = \sqrt{2}\alpha L_x/\hbar \propto \omega_P$$

SETUP



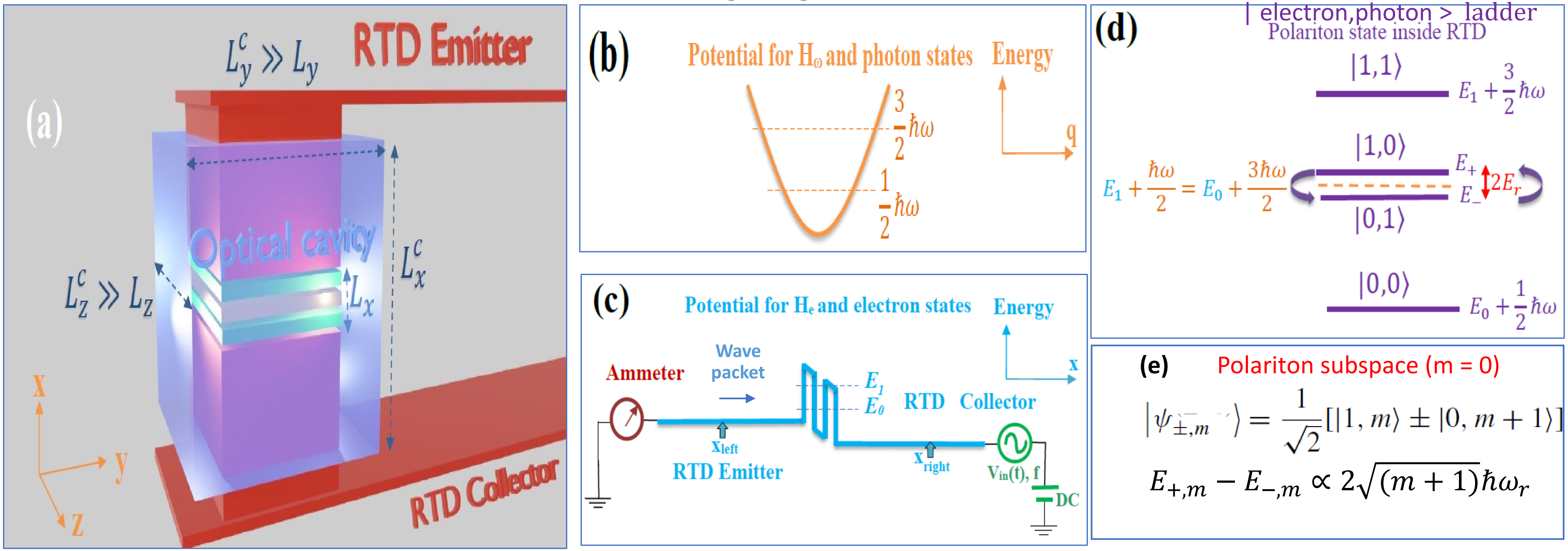
(a)
$L_y^c \gg L_y$
RTD Emitter
Optical cavity
$L_z^c \gg L_z$
L_x
L_x^c
x
y
z
RTD Collector

SETUP



(a)
RTD Emitter
$L_y^c \gg L_y$
Optical cavity
$L_z^c \gg L_z$
L_x
L_x^c
RTD Collector
x
y
z
(b)
Potential for H₀ and photon states
Energy
q
$\frac{3}{2}\hbar\omega$
$\frac{1}{2}\hbar\omega$
(c)
Potential for Hₑ and electron states
Energy
x
Ammeter
Wave packet
E_1
E_0
RTD
Collector
x_{left}
RTD Emitter
x_{right}
$V_{in}(t)$, f
DC

SETUP



(a)
$L_y^c \gg L_y$
RTD Emitter
Optical cavity
L_x^c
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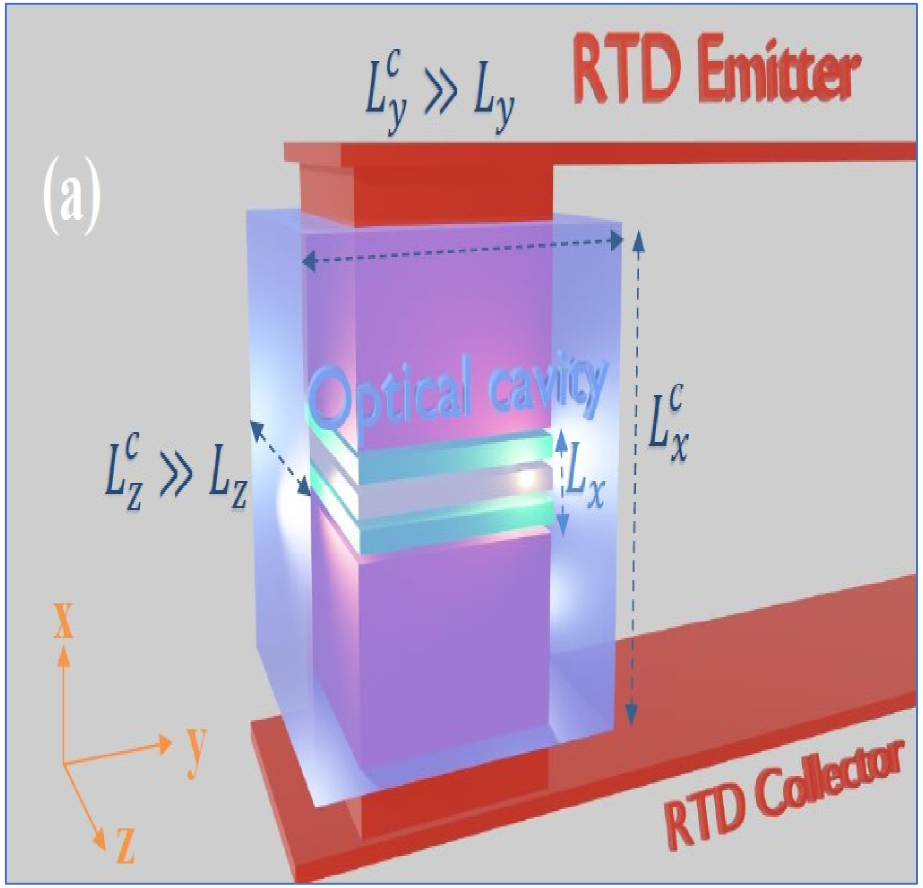
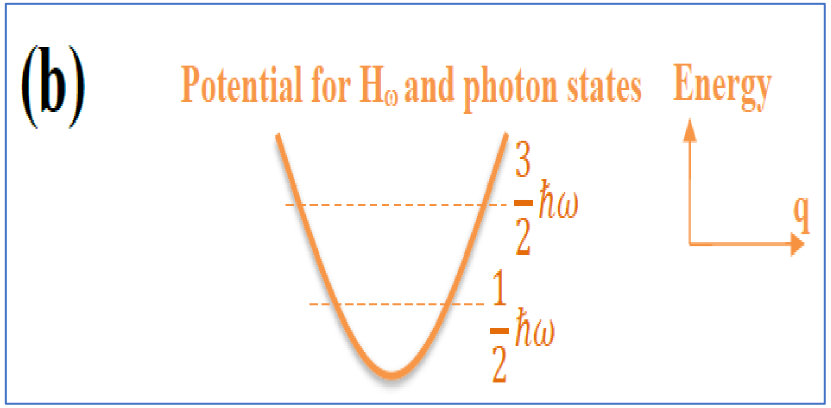
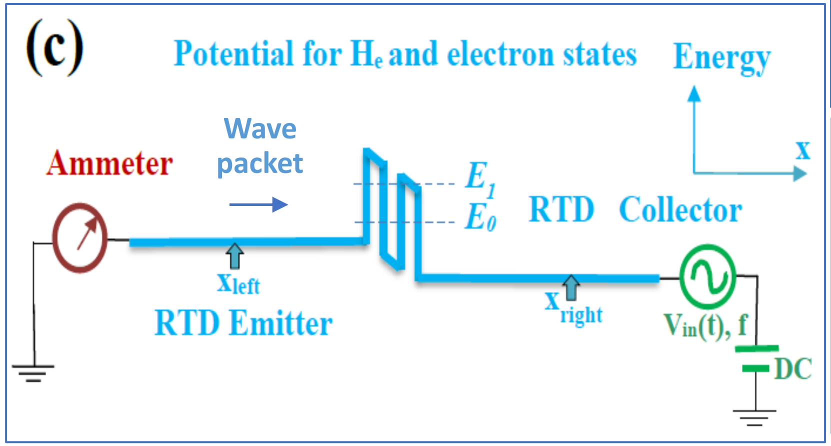
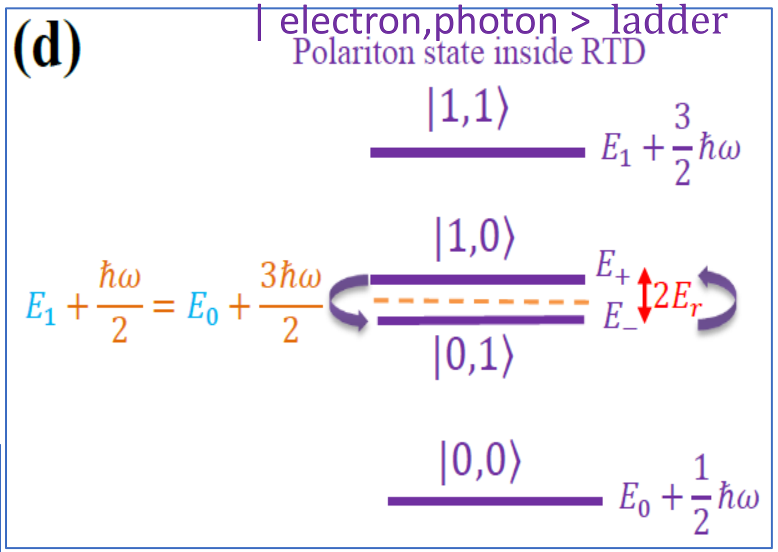
L_x
RTD Collector
x
y
z
(b)
Potential for H_ω and photon states
Energy
q
$\frac{3}{2}\hbar\omega$
$\frac{1}{2}\hbar\omega$
(c)
Potential for H_e and electron states
Energy
x
Ammeter
Wave packet
E_1
E_0
RTD
Collector
x_{left}
RTD Emitter
x_{right}
$V_{in}(t)$, f
DC
(d)
| electron,photon > ladder
Polariton state inside RTD
$|1,1\rangle$
$E_1 + \frac{3}{2}\hbar\omega$
$|1,0\rangle$
$E_1 + \frac{\hbar\omega}{2} = E_0 + \frac{3\hbar\omega}{2}$
E_+
$2E_r$
E_-
$|0,1\rangle$
$|0,0\rangle$
$E_0 + \frac{1}{2}\hbar\omega$
(e) Polariton subspace (m = 0)
$|\psi_{\pm,m}\rangle = \frac{1}{\sqrt{2}}[|1,m\rangle \pm |0,m+1\rangle]$
$E_{+,m} - E_{-,m} \propto 2\sqrt{(m+1)}\hbar\omega_r$

SETUP









(e) Polariton subspace (m = 0)

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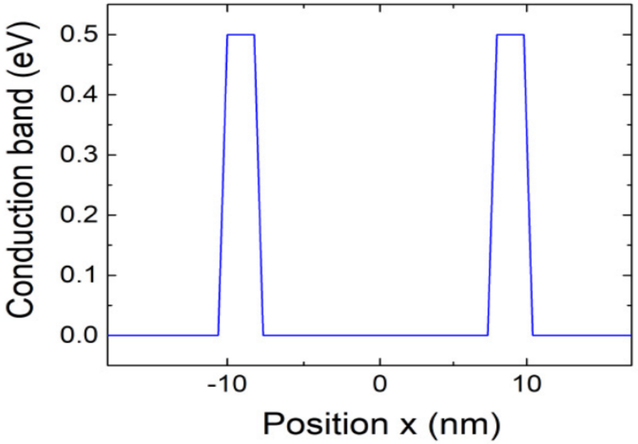
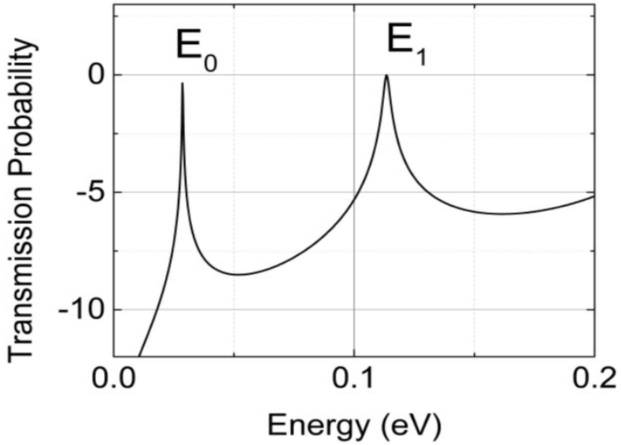




<u>AlAs/InGaAs/AlAs</u>

m_e = 0.041, $\mathcal{E}$ = 12.9, (L_B , L_x , L_B) = (2 , 16 , 2) nm

V_B = 500 meV , (E_0 , E_1)= (28 , 106) meV

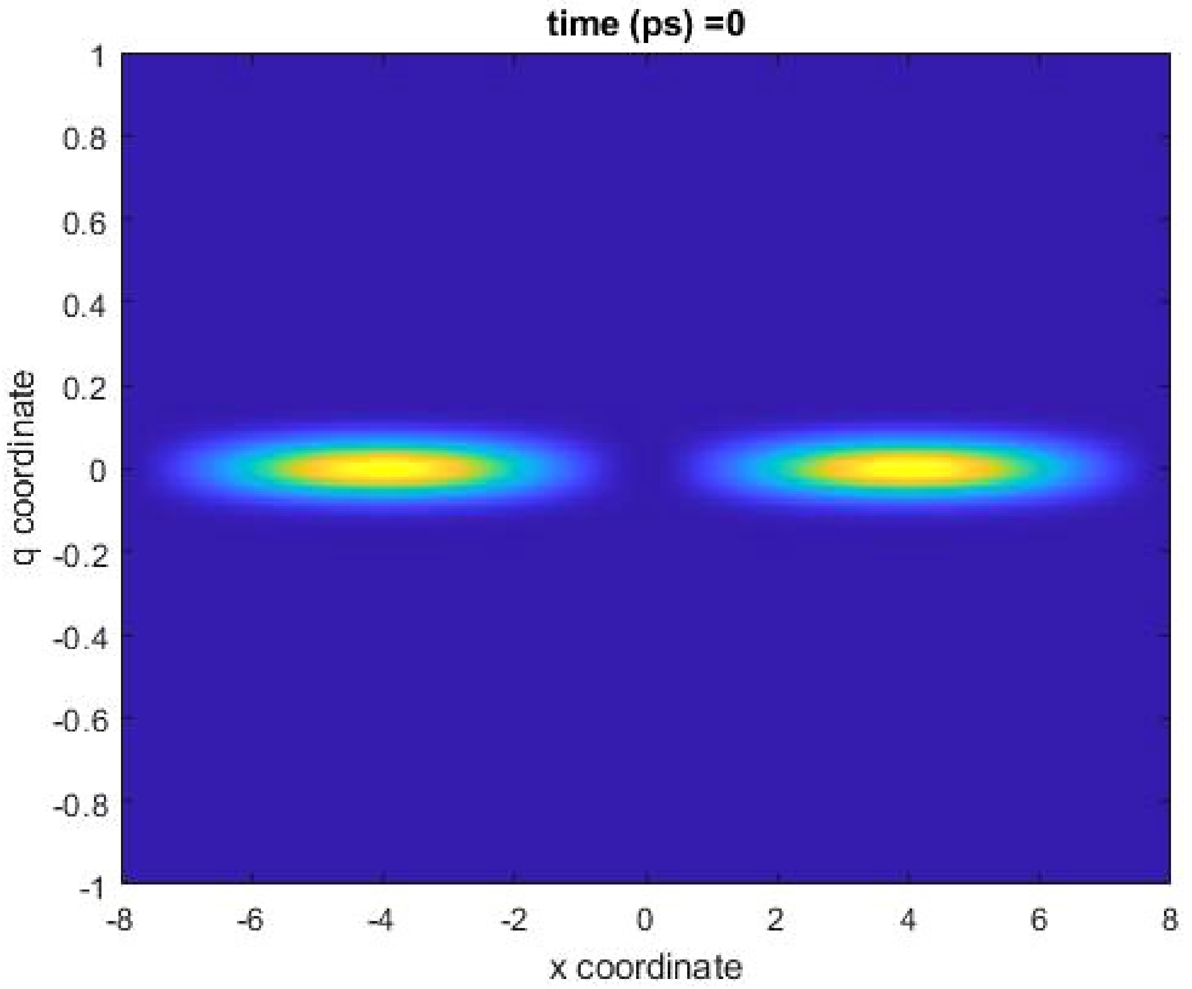
$\frac{\omega}{2\pi}$ = 19 THz , $L_{c,x} \cong$ μm, α = 1.33 meV/nm , $\gamma \cong 0.4$

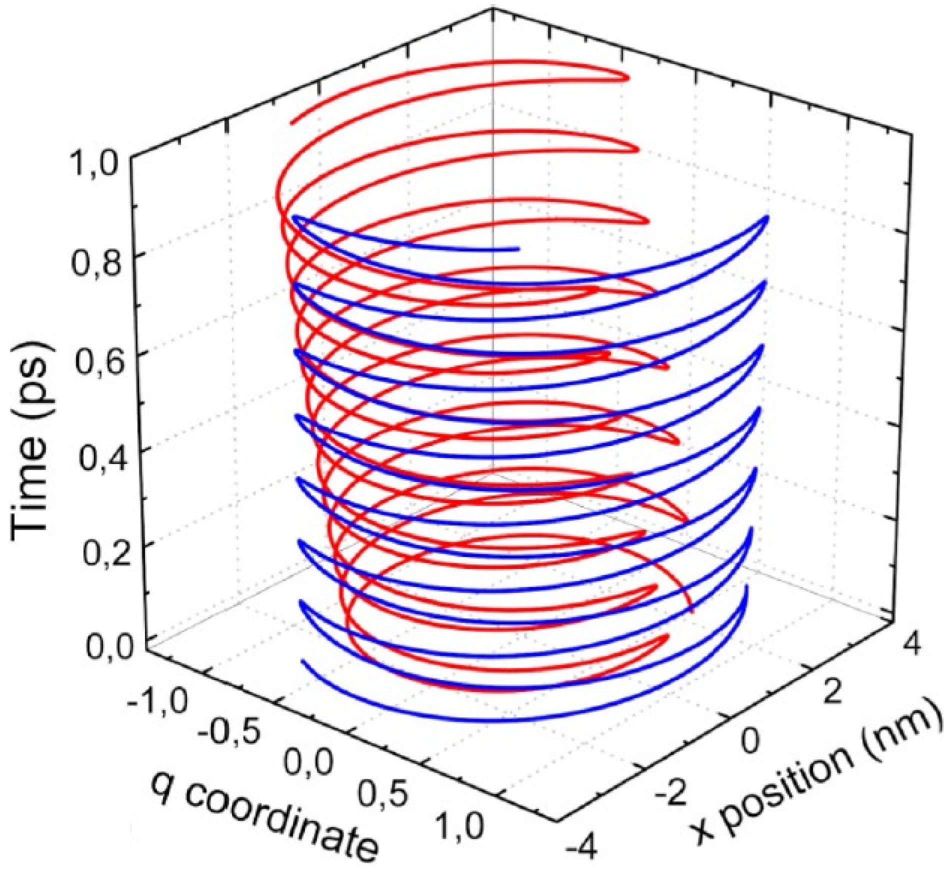
x_{left} = 520 nm, simulation box = 2 μm

[$\lambda_{cavity} \gg W_{device}$]

Closed system scenario (infinite well).

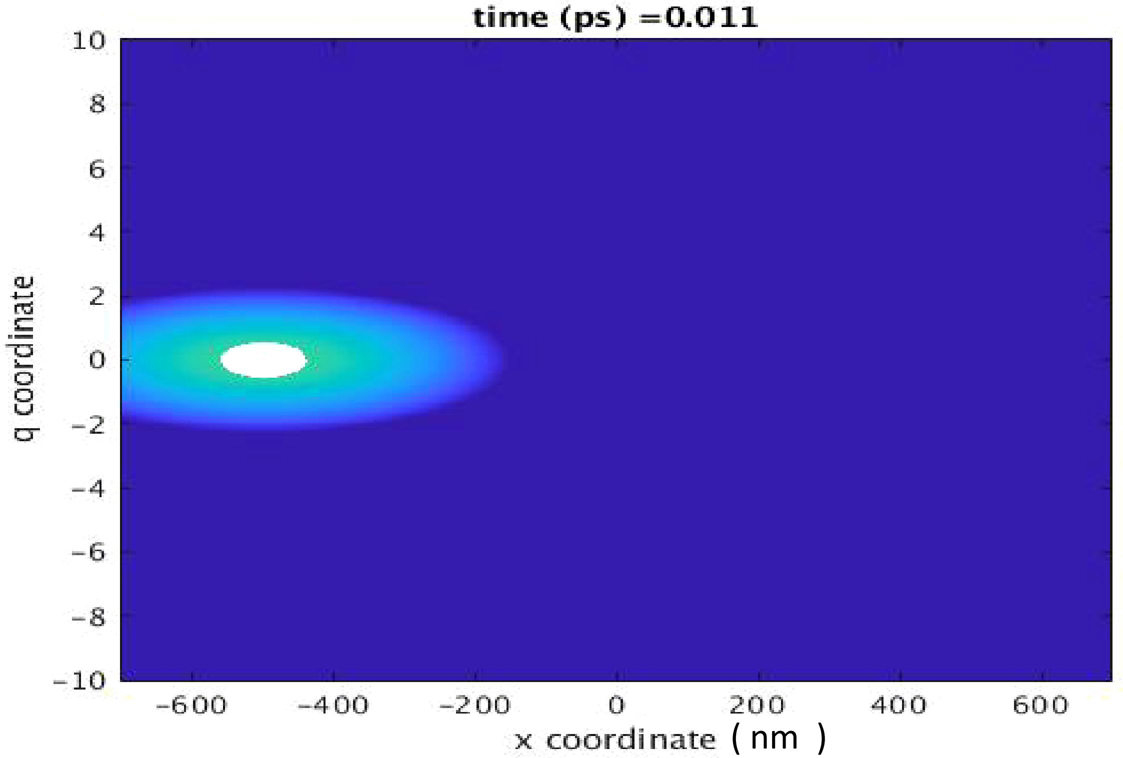
Jaynes-Cummings-like RWA solution from initial |1,0> state (double peak in *x*, single peak in *q*).

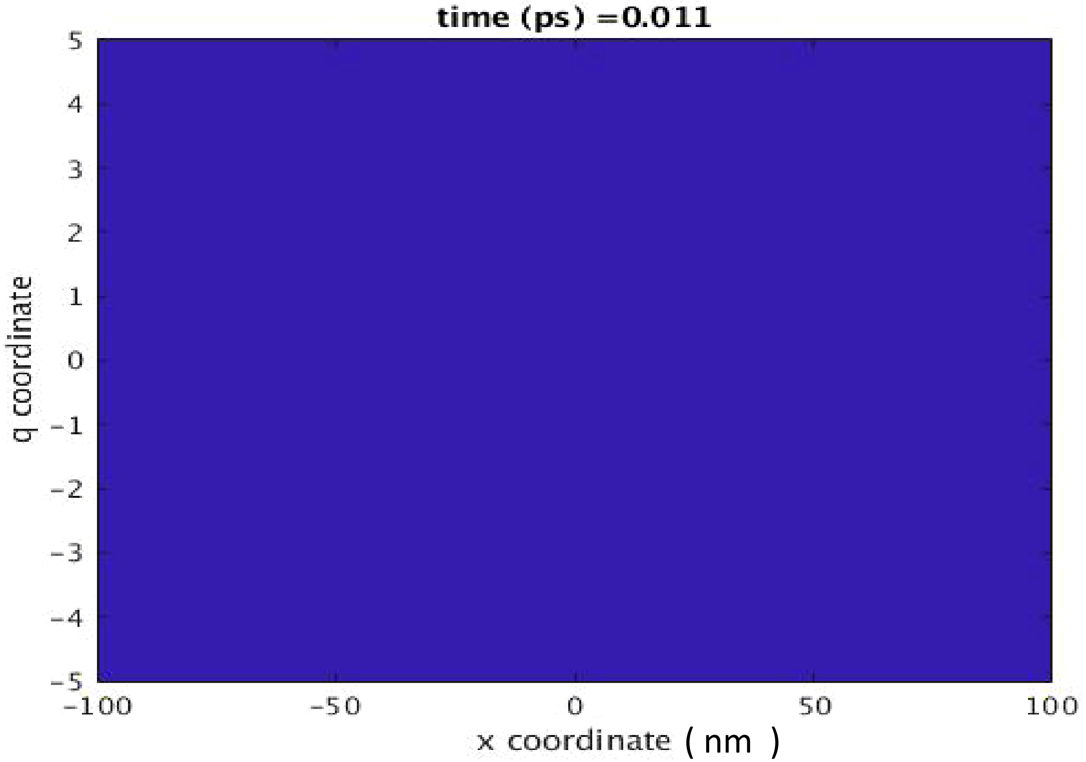


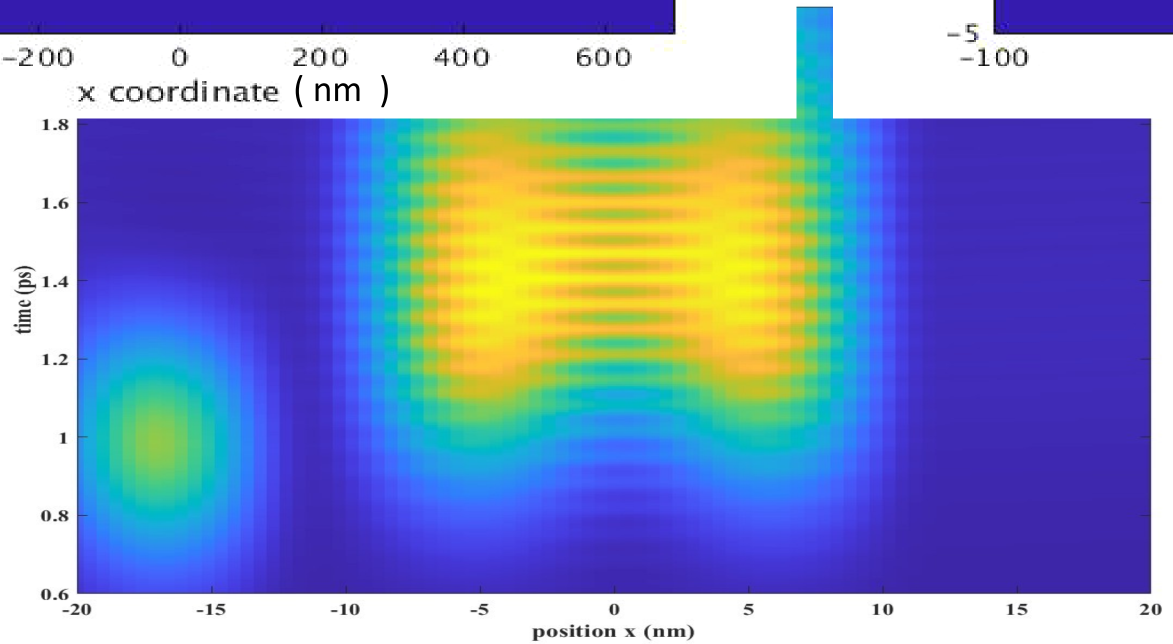


OK, but JC model not suitable for transport.

2D wavepacket with injection energy $E_{1,0}$. Nonzero coupling **only inside** active region.







OK, but "exact" model undoable for more electrons and/or more modes.

Born-Huang-like scheme

- Born-Huang : expand over well-known photon states ϕ(q), with wavepackets Φ(x,t).
- Previous 2D to 1D. More degrees of freedom via conditional wavefunctions.

$$\psi(x,q,t) = \sum_{m}^{N_\omega} \Phi_m(x,t)\phi_m^{(\omega)}(q)$$

(1D propagation only for electron degree *x*)

$$i\hbar\frac{\partial}{\partial t}\Phi_n(x,t) = [H_{xq,e}^{(D)} + \hbar\omega(n+1/2)]\Phi_n(x,t) + \alpha x[\sqrt{n+1}\Phi_{n+1}(x,t) + \sqrt{n}\Phi_{n-1}(x,t)]$$

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(if only 2 lowest levels)

$$\psi(x,q,t) = \Phi_0(x,t)\phi_0^{(\omega)}(q) + \Phi_1(x,t)\phi_1^{(\omega)}(q)$$

$$i\hbar\frac{\partial}{\partial t}\Phi_0(x,t) = \left[H_{xq,e}^{(D)} + \frac{\hbar\omega}{2}\right]\Phi_0(x,t) + \alpha x\Phi_1(x,t),$$

$$i\hbar\frac{\partial}{\partial t}\Phi_1(x,t) = \left[H_{xq,e}^{(D)} + \frac{3\hbar\omega}{2}\right]\Phi_1(x,t) + \alpha x\Phi_0(x,t)$$

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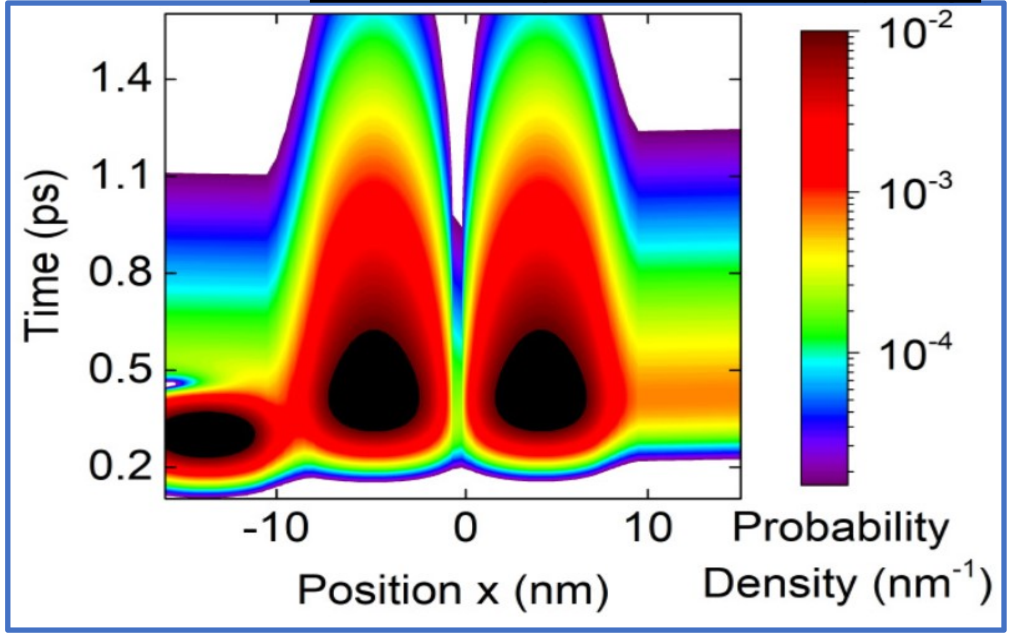
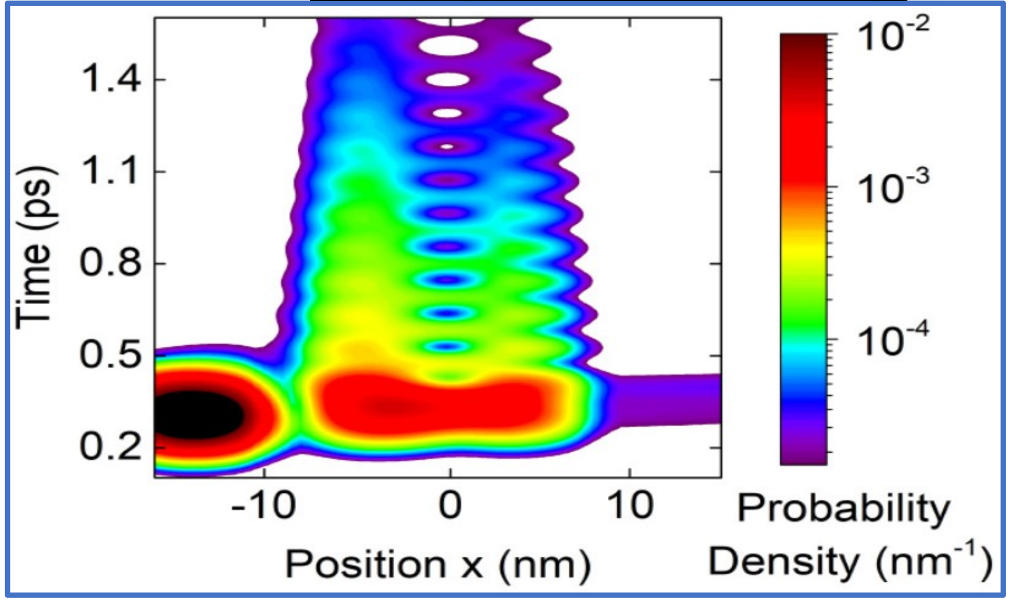
(without light-matter coupling)



(with light-matter coupling)



Displacement current

particle plus displacement current (external *f*)

$$\mathbf{J}(\mathbf{r},t) = \mathbf{J}_c(\mathbf{r},t) + \epsilon_0 \frac{\partial \mathbf{E}_{\parallel}(\mathbf{r},t)}{\partial t} + \epsilon_0 \frac{\partial \mathbf{E}_{\perp}(\mathbf{r},t)}{\partial t}$$

(Particle) (displacement)

Ramo-Shockley-Pellegrini Theorem

[total current from flux of distinct wavepackets (E, t_i , ...).
Bohmian velocities and conditional wave functions]

$$I^{(f)}(t) = \frac{e}{L_x} \sum_{j=1}^{N} \mathbf{v}_j(t) \cdot \mathbf{x}$$

$$\sum_{j=1}^{N(t)} \rightarrow \Gamma \int_{-\infty}^{t} dt_i \int_{-L_x/2}^{L_x/2} dx \int d\mathbf{W}_q |\psi(x, \mathbf{W}_q, t; t_i, E)|^2$$

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AC / DC displacement current coefficient

$$D^{(f)}(E,t) = \frac{I^{(f)}(E,t)}{e\Gamma}$$

(= T(E) if *f = 0*)
(DC Transmission coefficient)

$$= \frac{1}{L} \int_{-L_x/2}^{L_x/2} dx \int d\mathbf{W}_q \int_{-\infty}^{t} dt_i J_x(x,\mathbf{W}_q,t;t_i,E)$$

BITLLES SIMULATOR

Bohmian Interacting Transport in non-equiLibrium eLEctronic Structure

Displacement current

particle plus displacement current (external *f*)

$$\mathbf{J}(\mathbf{r},t) = \mathbf{J}_c(\mathbf{r},t) + \epsilon_0 \frac{\partial \mathbf{E}_{\parallel}(\mathbf{r},t)}{\partial t} + \epsilon_0 \frac{\partial \mathbf{E}_{\perp}(\mathbf{r},t)}{\partial t}$$

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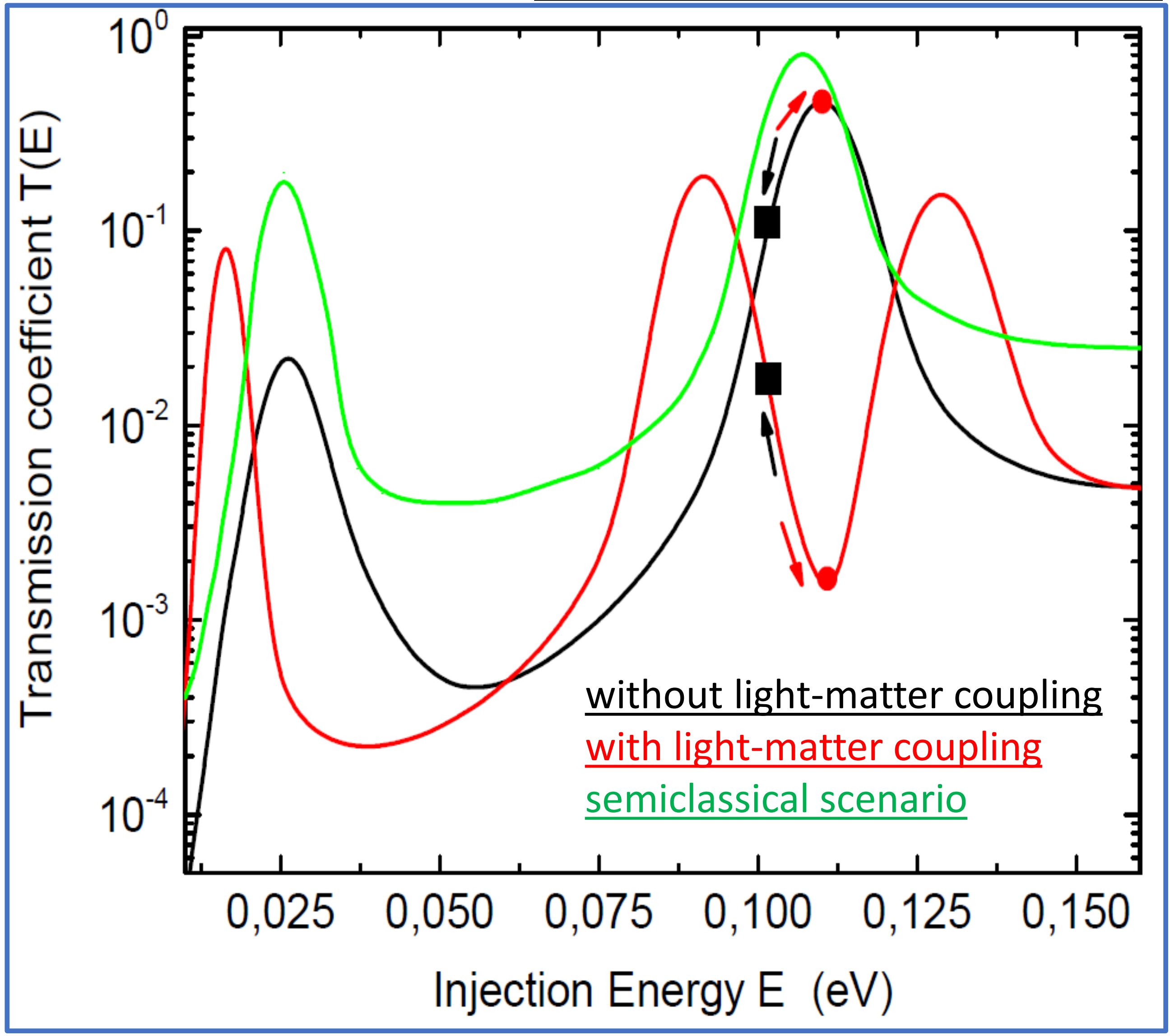
BITLLES SIMULATOR

Bohmian Interacting Transport in non-equiLibrium eLEctronic Structure

DC result (AC result elsewhere)



- polaritonic splitting of the first excited RTD state.
- ground state uncoupled.
- higher excited states coupled via other resonances.

SUMMARY

- Polariton signature not new neither unexpected : well-known in other platforms.
- 'Old-fashion' RTD + 'modern' microcavities : unexplored path for nanodevice engineering at THz.
- Theoretical side : need of new models at the strong coupling regime.
- Experimental side : RTD-based oscillators at THz need to improve output power.
- No photonics. Still electronics : no need of NDR.

Next steps

- Applying such models in simple structures like 'exciton polariton' (3D electron-hole-photon) or coupled QWs.
- Improving the initial approximations of these qualitative models.

THANK YOU for the attention!

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