Arrays of quantum dots or rings in a FIR-photon cavity

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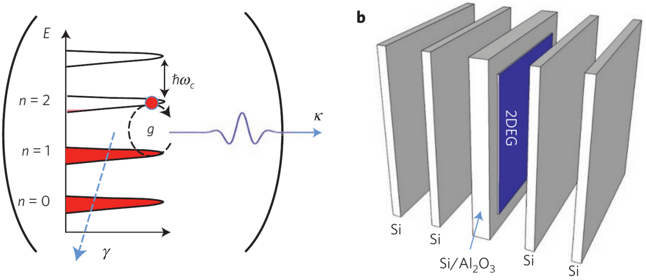
https://vidargudmundsson.org/Rann/Fyrirlestrar/10IWMP.pdf

Qi Zhang, *Nature Physics* **12**, 1005 (2016):

Collective non-perturbative coupling of 2D electrons with high-quality-factor terahertz cavity photons



- 2DEG in GaAs-AlGaAs heterostructure
- FIR photon cavity
- External magnetic field

QEDFT $\leftrightarrow$ QED-DFT-TP

Periodic 2DEG in magnetic field and FIR-photon cavity

$\Downarrow$

- Coulomb $+$ electron-photon interactions $\rightarrow$ DFT-functionals

- Coulomb interaction $\rightarrow$ DFT-functionals
- Electron-photon interaction $\rightarrow$ CI

$\Downarrow$

Cylindrical TE_{011} mode to promote high order magnetic transitions, no CM-electrical dipole modes

Model,(QED),(LSDA)

$$H = H_0 + V_{\rm H} + V_{\rm xc} + V_{\rm per} + H_\gamma^0 + H_\gamma^{\rm int}$$

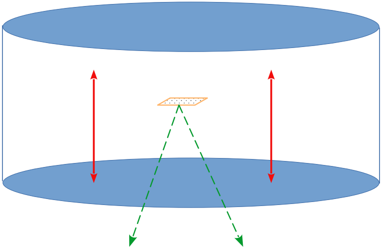
TE_{011} mode in cylindrical FIR cavity

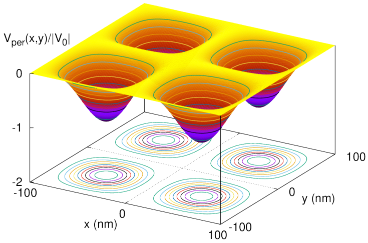
GaAs: $m^* = 0.067 m_e$, $\kappa = 12.4$, $g^* = -0.44$

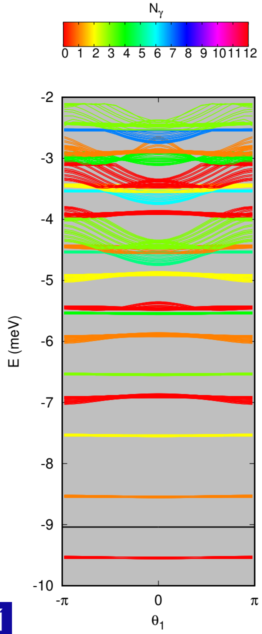
Para- and diamagnetic e-γ interactions

Long wavelength $\lambda >> L$

Basis: $\{|\mathrm{electron}\rangle \otimes |\mathrm{photon}\rangle\}$



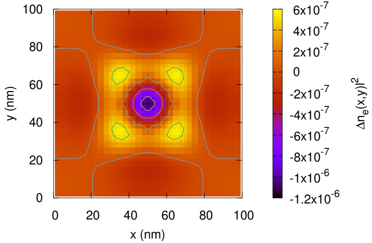


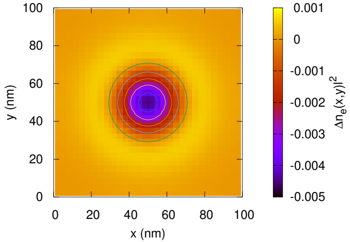


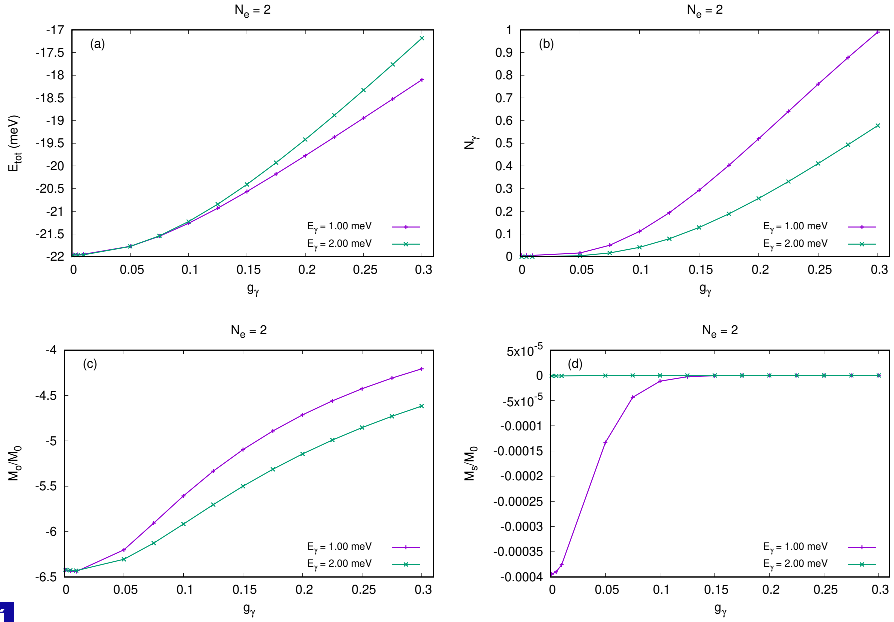
$$\Delta n_{\rm e} = n_{\rm e}(g_\gamma = 0.05) - n_{\rm e}(g_\gamma = 0.001)$$

$N_{\rm e} = 2, 3,\ pq = 2 \rightarrow B = 0.827$ T

$E_\gamma = 1.0$ meV







N_e = 2
(a)
E_tot (meV)
g_γ
E_γ = 1.00 meV
E_γ = 2.00 meV
N_e = 2
(b)
N_γ
g_γ
E_γ = 1.00 meV
E_γ = 2.00 meV
N_e = 2
(c)
M_o/M_0
g_γ
E_γ = 1.00 meV
E_γ = 2.00 meV
N_e = 2
(d)
M_s/M_0
g_γ
E_γ = 1.00 meV
E_γ = 2.00 meV

Excitation – short time modulation of the e-γ interaction

$$i\hbar\partial_t\rho^{\boldsymbol{\theta}}(t) = \left[H[\rho^{\boldsymbol{\theta}}(t)], \rho^{\boldsymbol{\theta}}(t)\right]$$

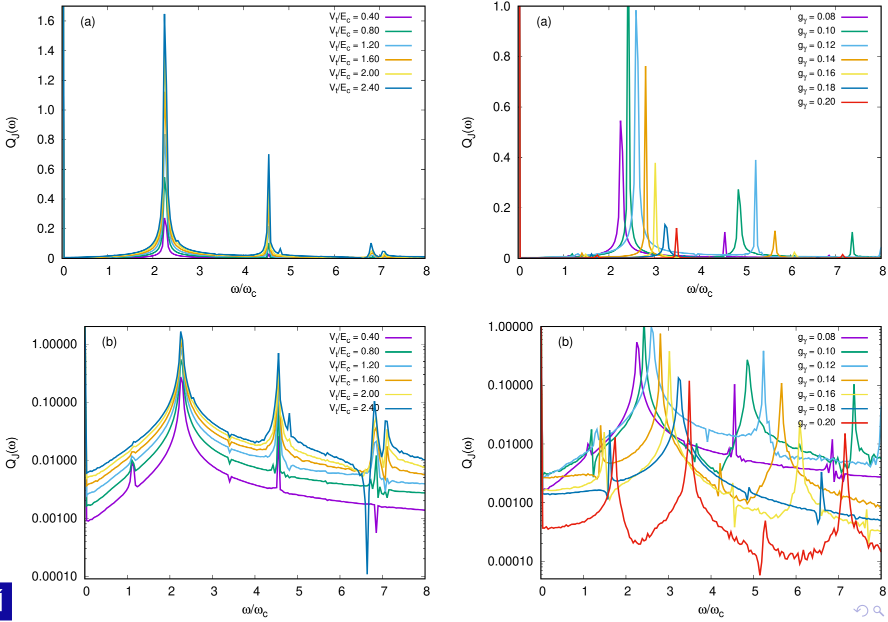
$$n_\sigma(\boldsymbol{r},t) = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi} d\boldsymbol{\theta} \sum_{\boldsymbol{\alpha\beta}} \phi^*_{\boldsymbol{\alpha\theta}\sigma}(\boldsymbol{r})\phi_{\boldsymbol{\beta\theta}\sigma}(\boldsymbol{r})\rho^{\boldsymbol{\theta}}_{\boldsymbol{\alpha}\sigma,\boldsymbol{\beta}\sigma}(t)$$

$$Q_J(t) = \frac{1}{2c\mathcal{A}}\int_{\mathcal{A}} d\boldsymbol{r}\left\{\boldsymbol{r}\times\boldsymbol{j}(\boldsymbol{r},t)\right\}\cdot\boldsymbol{e}_z,$$

$$\boldsymbol{j}_i(\boldsymbol{r},t) = \frac{-e}{m^*(2\pi)^2}\sum_{\boldsymbol{\alpha\beta}\sigma}\int_{-\pi}^{\pi} d\boldsymbol{\theta}\, \Re\left\{\phi^*_{\boldsymbol{\alpha\theta}\sigma}(\boldsymbol{r})\boldsymbol{\pi}_i\phi_{\boldsymbol{\beta\theta}\sigma}(\boldsymbol{r})\right\}\rho^{\boldsymbol{\theta}}_{\boldsymbol{\beta\theta}\sigma,\boldsymbol{\alpha\theta}\sigma}(t)$$

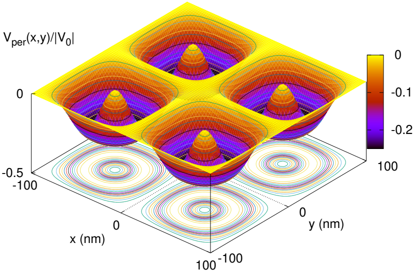
$$N_\gamma(t) = \frac{1}{(2\pi)^2}\sum_{\sigma}\int_{-\pi}^{\pi} d\boldsymbol{\theta}\,\mathrm{Tr}\left\{\rho^{\boldsymbol{\theta}}_\sigma(t)a^\dagger_\gamma a_\gamma\right\}$$

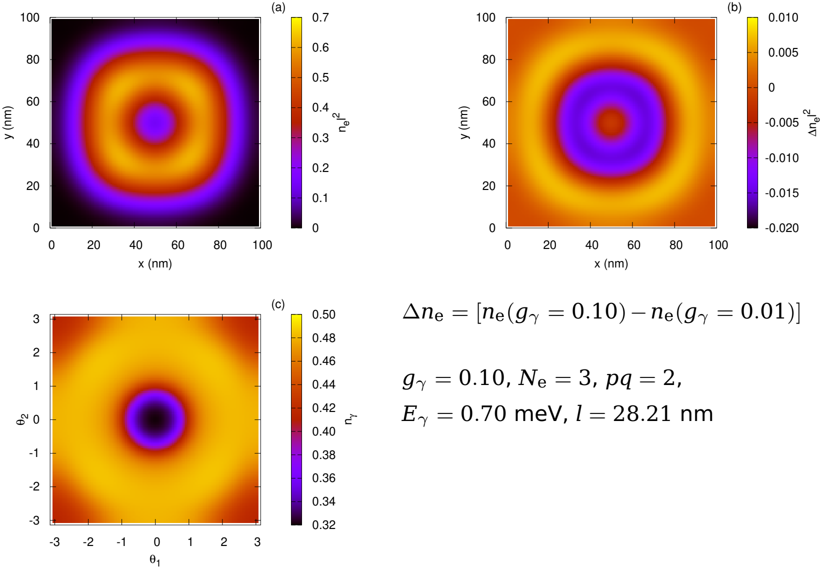
$pq = 2$, $N_\mathrm{e} = 1$, $E_\gamma = 1.4$ meV, $\hbar\omega_c = 1.429$ meV



Array of rings

- Changed energy spectrum
- Stronger inter-exchange forces than for dots
- We know e-γ-interactions tends to reduce Coulomb exchange forces

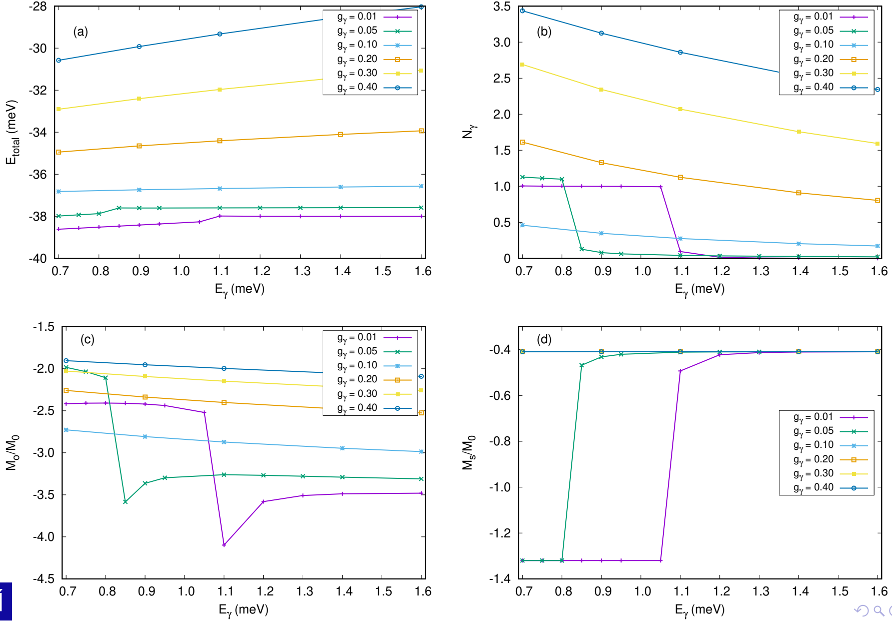




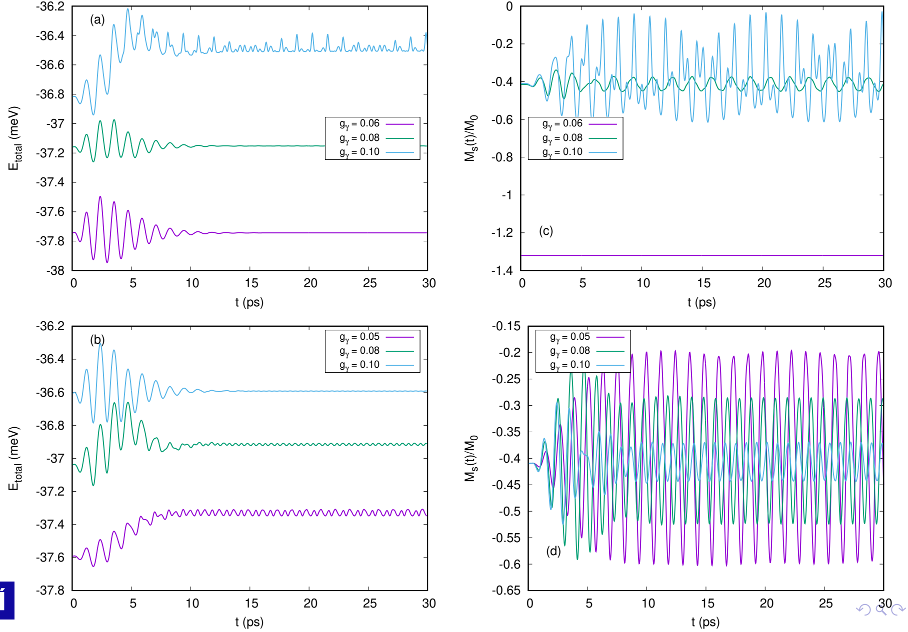
$$\Delta n_{\rm e} = [n_{\rm e}(g_\gamma = 0.10) - n_{\rm e}(g_\gamma = 0.01)]$$

$g_\gamma = 0.10$, $N_{\rm e} = 3$, $pq = 2$,
$E_\gamma = 0.70$ meV, $l = 28.21$ nm

$N_{\mathrm{e}} = 3$, $pq = 2$, $T = 1.0$ K, transition between spin-configurations



$N_e = 3$, $pq = 2$, $T = 1.0$ K, $E_\gamma = 0.7, 1.4$ meV, dynamic spin instability



Conclusions

- DFT + CI for a large 2D system in FIR-cavity and external magnetic field
- Charge polarization, γ-replicas
- Self-consistent (DFT + CI)-time-evolution $\rightarrow$ non-linear response
- High-order magnetic transitions
- 2-γ diamagnetic transitions most prominent
- e-γ-interactions $\rightarrow$ reduce Coulomb exchange
- FIR-cavity $\rightarrow$ transition between spin configurations
- (QED-DFT-TP – 3M CPU hr on 128core AMD nodes)

Collaborators - publications

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Hsi-Sheng Goan NTU, (TW)
Jeng-Da Chai NTU, (TW)
Nzar Rauf Abdullah SU, (IQ)
Chi-Shung Tang NUU, (TW)
Valeriu Moldoveanu NIMP, (RO)
Andrei Manolescu RU, (IS)

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Appendix QED

$$
\begin{aligned}
H = &\int d\boldsymbol{r}\, \psi^\dagger(\boldsymbol{r}) \left\{ \frac{\pi^2}{2m^*} + V(\boldsymbol{r}) \right\} \psi(\boldsymbol{r}) \\
&+ H_{\mathrm{EM}} + H_{\mathrm{Coul}} + H_{\mathrm{Z}} \\
&+ \frac{1}{c} \int d\boldsymbol{r}\, \boldsymbol{j}(\boldsymbol{r}) \cdot \boldsymbol{A}_\gamma + \frac{e^2}{2m^* c^2} \int d\boldsymbol{r}\, n_e(\boldsymbol{r}) A_\gamma^2
\end{aligned}
$$

$$
\boldsymbol{j} = -\frac{e}{2m^*} \left\{ \psi^\dagger \boldsymbol{\pi} \psi + \boldsymbol{\pi}^* \psi^\dagger \psi \right\}, \quad n_e = \psi^\dagger \psi
$$

$$
\boldsymbol{\pi} = \left(\boldsymbol{p} + \frac{e}{c} \boldsymbol{A}_{\mathrm{ext}} \right), \qquad \boldsymbol{A}_{\mathrm{ext}} = \frac{B}{2}(-y, x)
$$

$\boldsymbol{A}_\gamma$: the cavity vector field

$$\boldsymbol{A}_\gamma(\boldsymbol{r}) = \boldsymbol{e}_\phi \mathcal{A}_\gamma \left(a_\gamma^\dagger + a_\gamma\right) \left(\frac{r}{l}\right)$$

$$\begin{aligned} H_{\mathrm{int}} &= g_\gamma \hbar\omega_c \left\{lI_x + lI_y\right\} \left(a_\gamma^\dagger + a_\gamma\right) \\ &\quad + g_\gamma^2 \hbar\omega_c \mathcal{N} \left\{ \left(a_\gamma^\dagger a_\gamma + \frac{1}{2}\right) + \frac{1}{2}\left(a_\gamma^\dagger a_\gamma^\dagger + a_\gamma a_\gamma\right) \right\} \end{aligned}$$

$$\begin{aligned} l(I_x + I_y) &= \frac{m^*}{e} \int_{\boldsymbol{\mathcal{A}}} d\boldsymbol{r}\, \frac{l}{\hbar} \left[-j_x(\boldsymbol{r}) \left(\frac{y}{l}\right) + j_y(\boldsymbol{r}) \left(\frac{x}{l}\right) \right] \\ \mathcal{N} &= \int_{\boldsymbol{\mathcal{A}}} d\boldsymbol{r}\, n_{\mathrm{e}}(\boldsymbol{r}) \left(\frac{x^2 + y^2}{l^2}\right). \end{aligned}$$

$$g_\gamma = \left\{ \left(\frac{e\mathcal{A}_\gamma}{c}\right) \frac{l}{\hbar} \right\}, \quad l = (\hbar c/(eB))^{1/2}$$

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Appendix DFT - LSDA

$$n_e = n_\uparrow + n_\downarrow, \quad \zeta = (n_\uparrow - n_\downarrow)/n_e, \quad \nu(\boldsymbol{r}) = 2\pi l^2 n_e(\boldsymbol{r})$$

$$\epsilon_{\mathrm{xc}}^{B}(\nu,\zeta) = \epsilon_{\mathrm{xc}}^{\infty}(\nu) e^{-f(\nu)} + \epsilon_{\mathrm{xc}}^{0}(\nu,\zeta)(1 - e^{-f(\nu)})$$

$$f(\nu) = (3\nu/2) + 7\nu^4, \quad \epsilon_{\mathrm{xc}}^{\infty}(\nu) = -0.782\sqrt{\nu} e^2/(\kappa l)$$

$$\epsilon_{\mathrm{xc}}^{0}(\nu,\zeta) = \epsilon_{\mathrm{xc}}(\nu,0) + f^i(\zeta)\left[\epsilon_{\mathrm{xc}}(\nu,1) - \epsilon_{\mathrm{xc}}(\nu,0)\right]$$

$\epsilon_{\mathrm{xc}}(\nu,\zeta) = \epsilon_{\mathrm{x}}(\nu,\zeta) + \epsilon_{\mathrm{c}}(\nu,\zeta)$, with $\epsilon_{\mathrm{x}}(\nu,0) = -[4/(3\pi)]\sqrt{\nu}e^2/(kl)$, and

$$\epsilon_{\mathrm{x}}(\nu,1) = -[4/(3\pi)]\sqrt{2\nu}e^2/(kl)$$

$$f^i(\zeta) = \frac{(1+\zeta)^{3/2} + (1-\zeta)^{3/2} - 2}{2^{3/2} - 2}$$

$$\epsilon_c(\nu,\zeta) = a_0 \frac{1 + a_1 x}{1 + a_1 x + a_2 x^2 + a_3 x^3} Ry^*$$

$$x = \sqrt{r_s} = (2/\nu)^{1/4} (l/a_B^*)^{1/2}$$

$$V_{\mathrm{xc},\uparrow} = \frac{\partial}{\partial \nu}(\nu \epsilon_{\mathrm{xc}}) + (1-\zeta)\frac{\partial}{\partial \zeta}\epsilon_{\mathrm{xc}}$$
$$V_{\mathrm{xc},\downarrow} = \frac{\partial}{\partial \nu}(\nu \epsilon_{\mathrm{xc}}) - (1+\zeta)\frac{\partial}{\partial \zeta}\epsilon_{\mathrm{xc}}$$

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