



Electron-photon many-body systems

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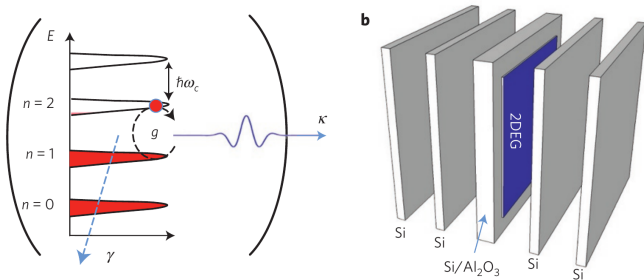
vidar@hi.is

NORDITA board meeting, Reykjavík

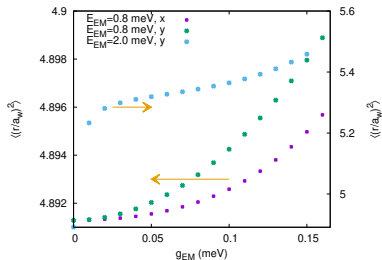
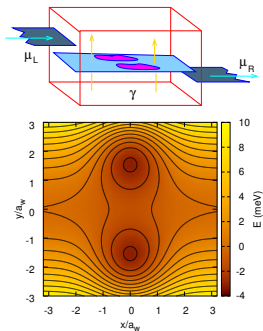
<https://vidargudmundsson.org/Rann/Fyrirlestrar/N-BMeeting-2023.pdf>

May 25, 2023

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



- Exact diagonalization, one photon mode
- $\hbar\omega = 0.8$ meV

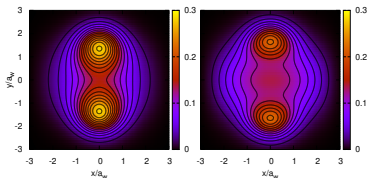
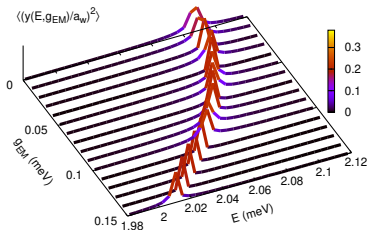
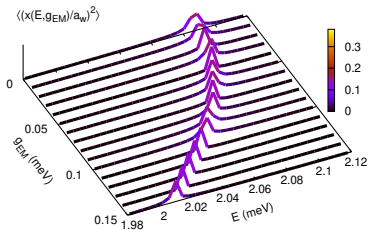
- 2 electrons, first photon replica
- Polarizability**

Real-time excitation

$$V_{\text{ext}}(\mathbf{r}, t) = V_t \left[\frac{\mathbf{r} \cdot \hat{\mathbf{e}}}{a_W^2} \right] \exp(-\Gamma t) \sin(\omega_1 t)$$

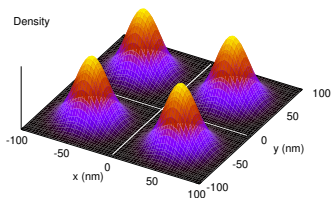
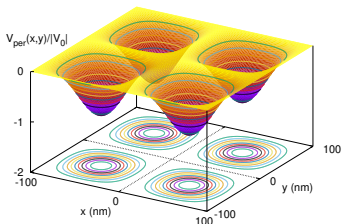


← Red-shift



Initial |16) – contributed |61)

Large electron system – 2DEG



- No exact diagonalization possible



- QED + DFT = QEDFT

- Use and adapt functional:

$E_{xc}^{GA}[n_e, \nabla n_e]$, proposed by Johannes Flick, [Simple](#)

[Exchange-Correlation Energy Functionals for Strongly Coupled Light-Matter Systems based on the Fluctuation-Dissipation Theorem](#),

Phys. Rev. Lett. **129**, 143201 (2022)

Model and EM functional, (QED)

$$H = H_0 + H_{Zee} + V_H + V_{\text{per}} + V_{\text{xc}} + V_{\text{xc}}^{\text{EM}} \quad (\text{LSDA})$$

$$E_{\text{xc}}^{\text{GA}}[n_e, \nabla n_e] = \frac{1}{16\pi} \sum_{\alpha=1}^{N_p} |\lambda_{\alpha}|^2 \int d\mathbf{r} \frac{\hbar\omega_p(\mathbf{r})}{\sqrt{(\hbar\omega_p(\mathbf{r}))^2/3 + (\hbar\omega_g(\mathbf{r}))^2 + \hbar\omega_{\alpha}}}$$

(AC-FDT)

$$(\hbar\omega_g)^2 = C \left| \frac{\nabla n_e}{n_e} \right|^4 \frac{\hbar^2}{m^{*2}}$$

$$(\hbar\omega_p(q))^2 = (\hbar\omega_c)^2 + \frac{2\pi n_e^2}{m^* \kappa} q + \frac{3}{4} v_F^2 q^2$$

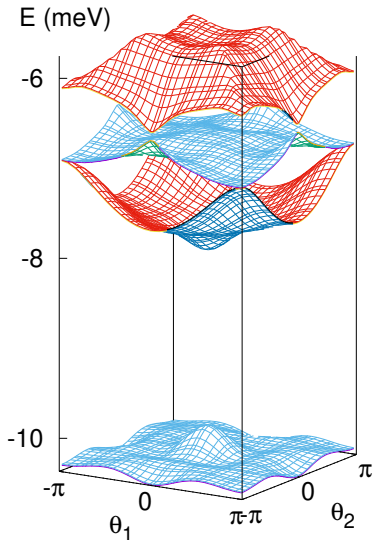
$$\omega_c = \left(\frac{eB}{m^* c} \right), \quad l^2 = \left(\frac{\hbar c}{eB} \right)$$

Select $N_p = 1$, $\hbar\omega_{\alpha} = 1.0$ meV, $L = 100$ nm, $m^* = 0.067m_e$, $\kappa = 12.4$, $g^* = 0.44$, and $q \approx k_F/6 \approx |\nabla n_e|/(6n_e)$. $\lambda_{\alpha}l$ is measured in $\text{meV}^{1/2}$

Commensurability

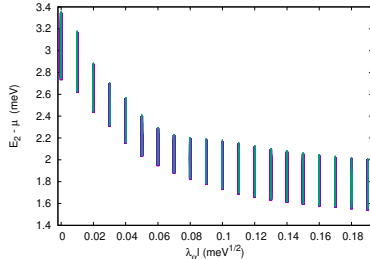
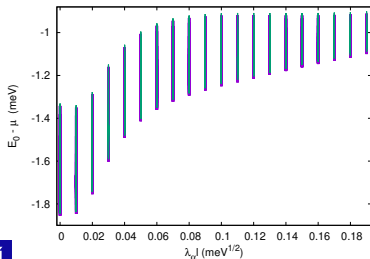
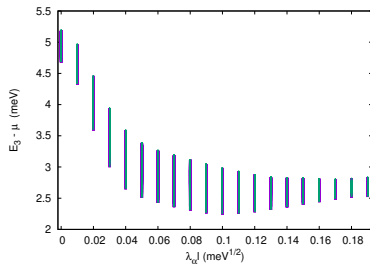
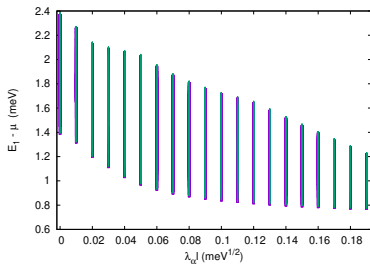
- L and l are competing length scales - Hofstadter problem:
Phys. Rev. B **14**, 2239 (1976)
- Magnetic flux through unit cell: $B\mathcal{A} = pq\Phi_0$, $\Phi_0 = hc/e$,
 $p, q \in \mathbf{N}$

$$\begin{aligned} N_e = 2, pq = 1 &\quad \rightarrow \\ \lambda_\alpha l = 0.050 \text{ meV}^{1/2} \\ \mu = -8.954 \text{ meV} \\ T = 1.0 \text{ K} \\ \hbar\omega_\alpha = 1.0 \text{ meV} \\ E_{Zee} = 1.053 \times 10^{-2} \text{ meV} \end{aligned}$$

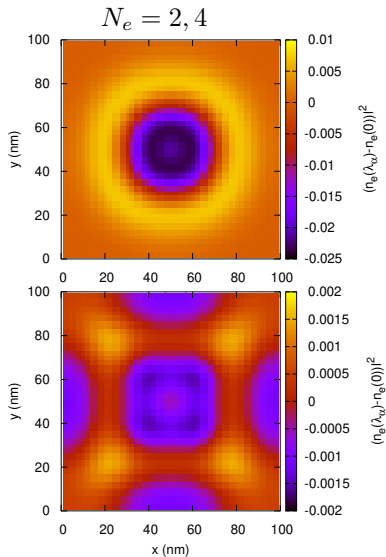
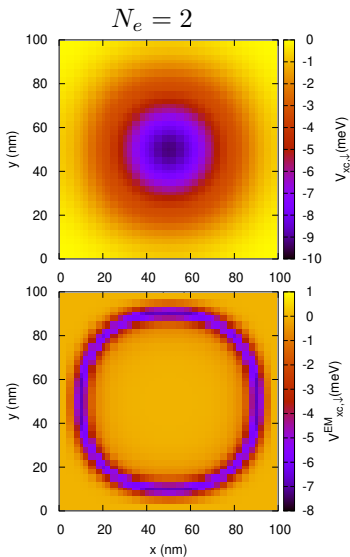


Polaritons emerge, $pq = 1$

Phys. Rev. B 106, 115308 (2022)



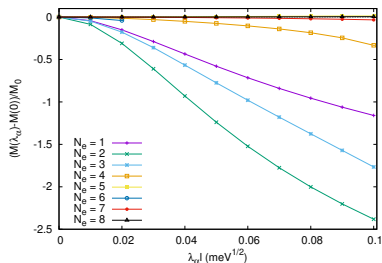
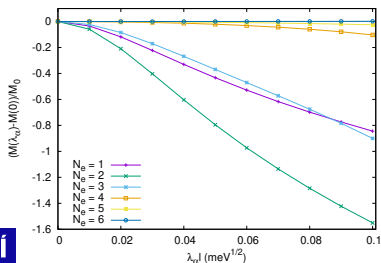
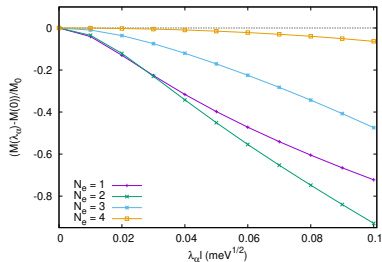
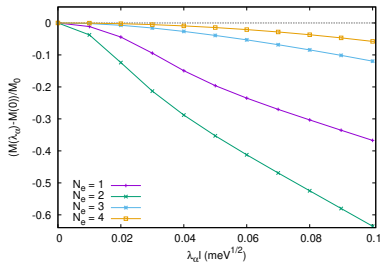
$$V_{xc}, V_{xc}^{EM}, \quad [n_e(\lambda_\alpha) - n_e(0)], \quad pq = 4, \quad \lambda_\alpha l = 0.050 \text{ meV}^{1/2}$$



Cavity-photon influence on orbital magnetization

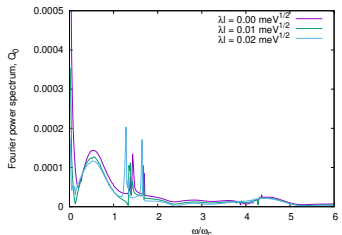
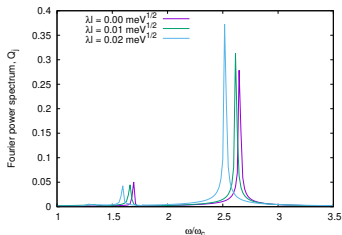
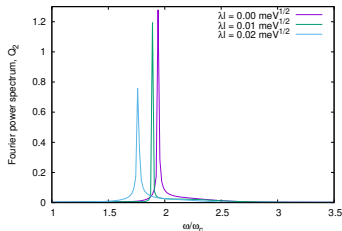
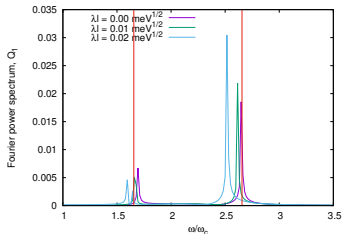
$pq = 1, 3$

$pq = 2, 4$



Real-time excitation \rightarrow red-shift of modes

$$pq = 4, N_e = 2, Q_1, Q_2, Q_j, Q_0, \text{ arXiv:2305.11544}$$



Summary

- Exact diagonalization
↔ small systems
- Open systems ↔ transport,
high-order single-mode QED
- Large 2DEG ↔ QEDFT
(GGA)
- e - γ influence on
magnetization, total energy
- Real-time excitations ↔
red-shift of collective
oscillations
- Andrei Manolescu (RU)
- Valeriu Moldoveanu (NIMP)
- Nzar Rauf Abdullah (US,
KUST)
- Chi-Shung Tang (NUU)
- Vram Mughnetsyan (YSU)

Icelandic Infrastructure Fund,
ihpc.is, UI, RU, RCP, MOST
Taiwan, ASCS

Appendix QED

$$H = \int d\mathbf{r} \psi^\dagger(\mathbf{r}) \left\{ \frac{\pi^2}{2m^*} + V(\mathbf{r}) \right\} \psi(\mathbf{r}) \\ + H_{\text{EM}} + H_{\text{Coul}} + H_Z \\ + \frac{1}{c} \int d\mathbf{r} \mathbf{j}(\mathbf{r}) \cdot \mathbf{A}_\gamma + \frac{e^2}{2m^*c^2} \int d\mathbf{r} n_e(\mathbf{r}) A_\gamma^2$$

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

with

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

\mathbf{A}_γ : the cavity vector field

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Appendix DFT - LSDA

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

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

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

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

$$\epsilon_{xc}(\nu, \zeta) = \epsilon_x(\nu, \zeta) + \epsilon_c(\nu, \zeta), \text{ with } \epsilon_x(\nu, 0) = -[4/(3\pi)]\sqrt{\nu}e^2/(kl), \text{ and} \\ \epsilon_x(\nu, 1) = -[4/(3\pi)]\sqrt{2\nu}e^2/(kl)$$

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

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

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

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

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

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Appendix AC-FDT

J. Flick PRL 129, 143201 (2022), Dipole approximation:

$$\hat{H}_{\text{int}} = \sum_{\alpha=1}^{N_p} \frac{1}{2} \left\{ (\boldsymbol{\lambda}_{\alpha} \cdot \mathbf{R})^2 - \omega_{\alpha} \hat{q}_{\alpha} \boldsymbol{\lambda}_{\alpha} \cdot \mathbf{R} \right\}, \quad \hat{q}_{\alpha} = \sqrt{\frac{1}{2\omega_{\alpha}}} (\hat{a}_{\alpha}^{\dagger} + \hat{a}_{\alpha})$$

$$\mathbf{R} = e \int d\mathbf{r} \mathbf{r} n_e(\mathbf{r}), \quad \boldsymbol{\lambda}_{\alpha} = 4\pi S(\mathbf{k}_{\alpha} \cdot \mathbf{R}) \hat{\mathbf{e}}_{\alpha}$$

$$U = \frac{1}{2} \iint d\mathbf{r} d\mathbf{r}' \left[\frac{e^2}{4\pi\epsilon} \frac{1}{|\mathbf{r} - \mathbf{r}'|} + \sum_{\alpha=1}^{N_p} (\boldsymbol{\lambda}_{\alpha} \cdot \mathbf{r})(\boldsymbol{\lambda}_{\alpha} \cdot \mathbf{r}') \right] n(\mathbf{r})n(\mathbf{r}') \\ + \frac{1}{2} \sum_{\alpha=1}^{N_p} \int d\mathbf{r} (\boldsymbol{\lambda}_{\alpha} \cdot \mathbf{r})^2 n(\mathbf{r})$$

$$E_c^{(1)} = \frac{1}{2\pi} \int_0^1 d\gamma \int d\mathbf{r} \sum_{\alpha=1}^{N_p} \omega_{\alpha} (\boldsymbol{\lambda}_{\alpha} \cdot \mathbf{r}) \int d\omega [\chi_{n,\gamma}^{q\alpha}(\mathbf{r}, i\omega) - \chi_{n,0}^{q\alpha}(\mathbf{r}, i\omega)]$$

$$E_c^{(2)} = -\frac{1}{2\pi} \int_0^1 d\gamma \int d\mathbf{r} \left[\frac{e^2}{4\pi\epsilon} \frac{1}{|\mathbf{r} - \mathbf{r}'|} + \sum_{\alpha=1}^{N_p} (\boldsymbol{\lambda}_{\alpha} \cdot \mathbf{r})(\boldsymbol{\lambda}_{\alpha} \cdot \mathbf{r}') \right] \\ \times \int d\omega [\chi_{n,\gamma}^n(\mathbf{r}, i\omega) - \chi_{n,0}^n(\mathbf{r}, i\omega)]$$

...

$$\alpha_{\mu,\nu}(i\omega) = 2 \sum_{ia} \frac{(\epsilon_a - \epsilon_e) \langle \phi_a | r_{\mu} | \phi_i \rangle \langle \phi_i | r_{\nu} | \phi_a \rangle}{(\epsilon_a - \epsilon_i)^2 + \omega^2}$$

$$\rightarrow \alpha(i\omega) = \frac{1}{4\pi} \int d\mathbf{r} \frac{\omega_p(\mathbf{r})}{\omega_p^2(\mathbf{r})/3 + \omega_g^2(\mathbf{r}) + \omega^2}$$

(compare to G. Mahan, chapter 4 for the last step)

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