Modeling static and dynamical properties of a 2DEG in an external magnetic field and a FIR-photon cavity

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https://vidar.hi.is/Rann/Fyrirlestrar/NTU-March-2024.pdf

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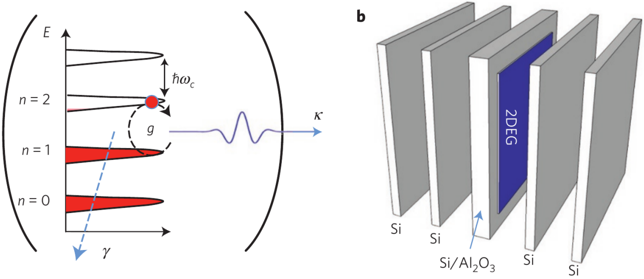
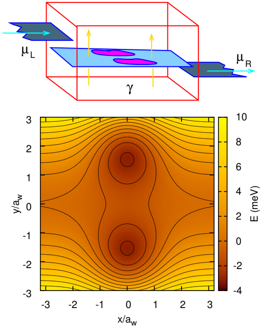
Qi Zhang, *Nature Physics* **12**, 1005 (2016):

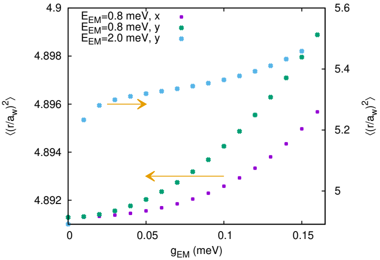
Collective non-perturbative coupling of 2D electrons with high-quality-factor terahertz cavity photons



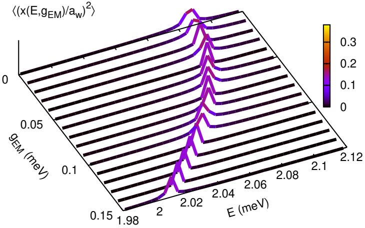
- 2DEG in GaAs-AlGaAs heterostructure
- FIR photon cavity
- External magnetic field

Gudmundsson et al. Annalen der Physik **528**, 394 (2016):





- Exact diagonalization, one photon mode
- $\hbar\omega = 0.8$ meV
- 2 electrons, first photon replica
- **Polarizability**

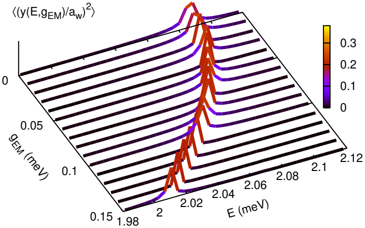


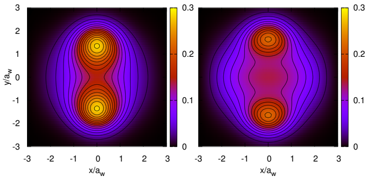
Real-time excitation

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

$\downarrow$

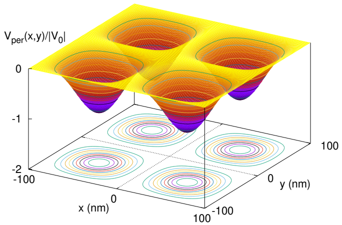
$\leftarrow$ Red-shift

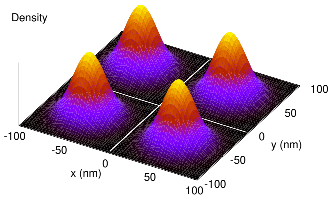




Initial $|16)$ – contributed $|61)$

Large electron system – 2DEG





- No exact diagonalization possible, (no CI)

$\downarrow$

- QED + DFT = QEDFT
- Use and adapt functional: $E_{\text{xc}}^{\text{GA}}[n_e, \boldsymbol{\nabla} n_e]$, proposed by Johannes Flick, Simple Exchange-Correlation Energy Functionals for Strongly Coupled Light-Matter Systems based on the Fluctuation-Dissipation Theorem, *PRL.* **129**, 143201 (2022)

Model and EM functional,(QED)

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

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

(AC-FDT)

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

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

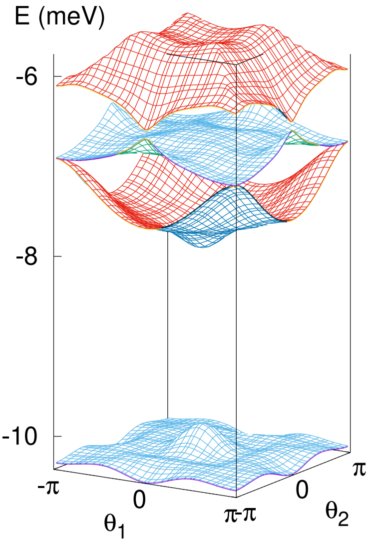
$$\omega_c = \left(\frac{eB}{m^*c}\right), \quad l^2 = \left(\frac{\hbar c}{eB}\right)$$

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

Commensurability

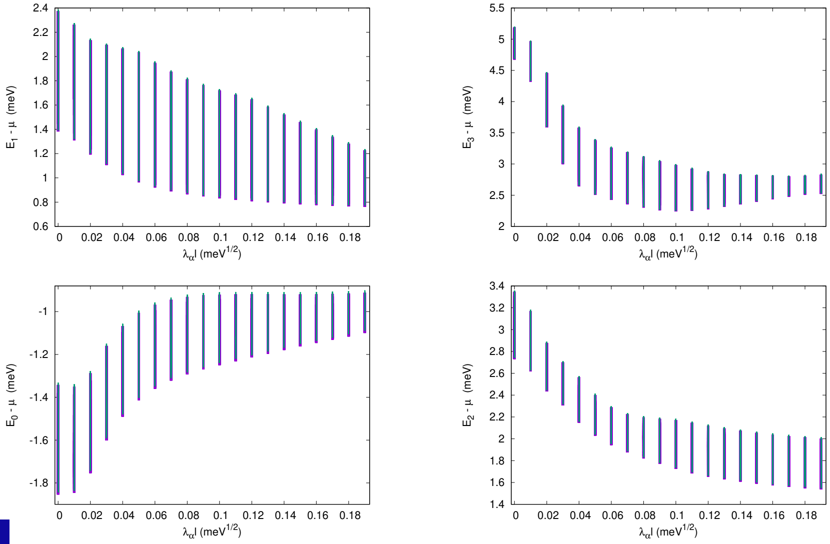
- L and l are competing length scales - Hofstadter problem: *Phys. Rev. B* **14**, 2239 (1976)
- Magnetic flux through unit cell: $B\mathcal{A} = pq\Phi_0$, $\Phi_0 = hc/e$, $p, q \in \boldsymbol{N}$

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

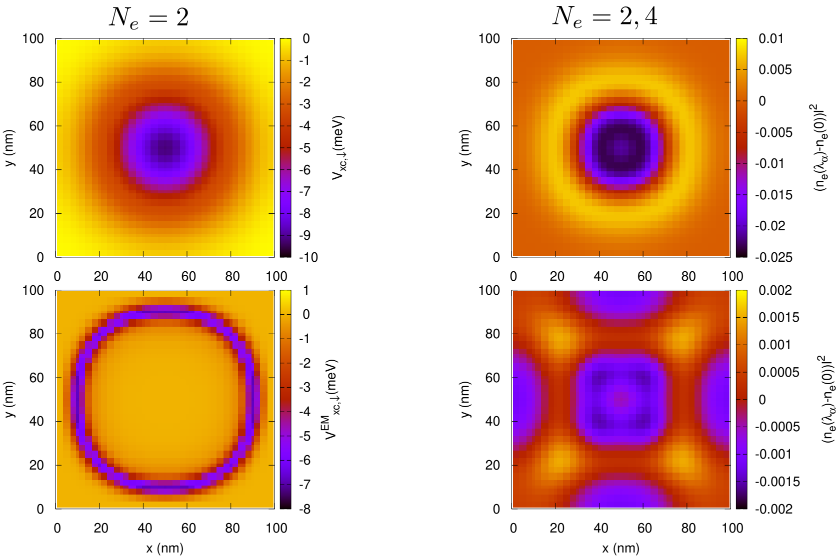


Polaritons emerge, $pq = 1$

Phys. Rev. **B** 106, 115308 (2022)

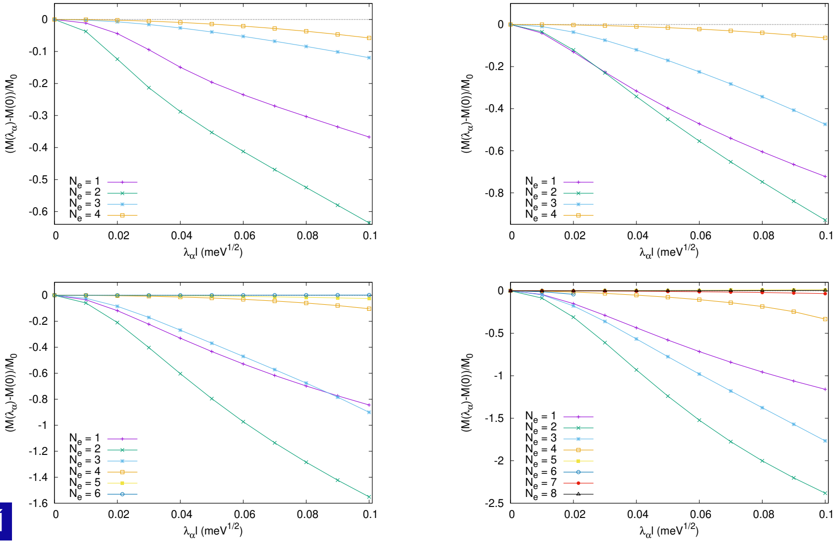


$V_{\rm xc}$, $V_{\rm xc}^{\rm EM}$, $[n_e(\lambda_\alpha) - n_e(0)]$, $pq = 4$, $\lambda_\alpha l = 0.050$ meV$^{1/2}$



Cavity-photon influence on orbital magnetization

$pq = 1, 3$ $pq = 2, 4$



Reall-time excitation → nonequilibrium (PRB **108**, 115306 (2023))

$$H(t) = H_{\rm stat} + V^{\rm ext}(\boldsymbol{r},t)$$

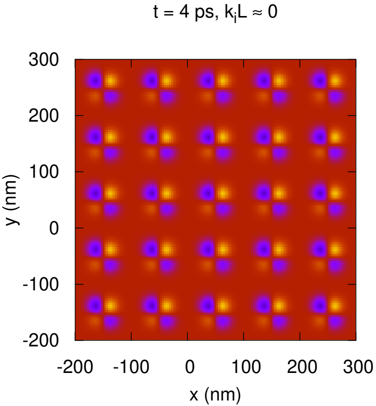
$$V^{\rm ext}(\boldsymbol{r},t) = V_{\rm t}\left\{(\Gamma t)^2 e^{-\Gamma t}\right\}\left[\cos{(k_y y)}\cos{(\Omega t)} \pm \cos{(k_x x)}\sin{(\Omega t)}\right]$$

$$i\hbar\partial_t\rho(t) = [H[\rho(t)],\rho(t)]$$

$\boldsymbol{k} \neq 0$ breaks the lattice symmetry → extend the Hilbert space basis:

$\{|\boldsymbol{\alpha},\sigma\rangle\}$ at each Brillouin point $\boldsymbol{\theta}$ → $\{|\boldsymbol{\alpha},\boldsymbol{\theta},\sigma\rangle\}$

Induced density



Calculate averages $\langle \hat{Q}_i \rangle = \mathrm{Tr}\{\hat{Q}_i \rho(t)\}$ for:

Dipole operators:
$\hat{Q}_1 = \hat{x}$ or $\hat{Q}_1 = \hat{y}$

Quadrupole:
$\hat{Q}_2 = \hat{yx} - \langle \hat{y} \rangle \langle \hat{x} \rangle$

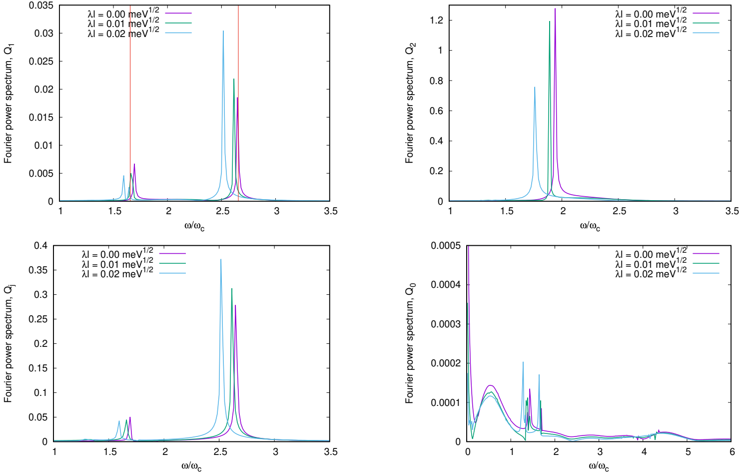
Monopole:
$\hat{Q}_0 =$
$\hat{x}^2 + \hat{y}^2 - \langle \hat{x} \rangle^2 - \langle \hat{y} \rangle^2$

Rotational mode:

$$Q_j = \frac{1}{l^2 \omega_c} \langle i(\boldsymbol{r} \times \dot{\boldsymbol{r}}) \cdot \hat{\boldsymbol{z}} \rangle$$

Real-time excitation → red-shift of modes

$pq = 4, N_e = 2, \quad Q_1, \quad Q_2, \quad Q_j, \quad Q_0,$ *PRB* **108**, 115306 (2023)



What is missing? $\rightarrow$ where are we heading

- No explicit photons
- Need Rabi resonances
- Need higher order photon processes

- QEDFT $\rightarrow$ QED-DFT-TP*
- Basis states: $|\boldsymbol{\alpha}, \boldsymbol{\theta}, \sigma, n\rangle = |\boldsymbol{\alpha}, \boldsymbol{\theta}, \sigma\rangle \otimes |n\rangle$
- Designed cavity modes

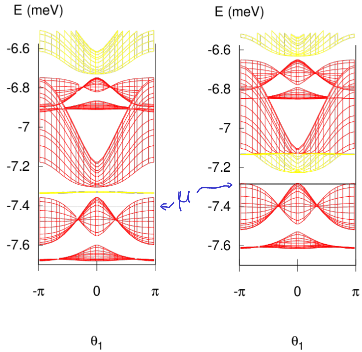
Quantized FIR-cavity field interacting with the electron current- and charge density from DFT

*(J. Malave et al., J. of Chem. Phys. **157**, 194106 (2022))

Photon content ↔ Rabi resonances

The projection of the energy spectra on one $\bar{\Theta}$ variable

only a part of the spectra shown



$g^{EM} = 0.01$ $\qquad$ $g^{EM} = 0.10$

$pq = 3$

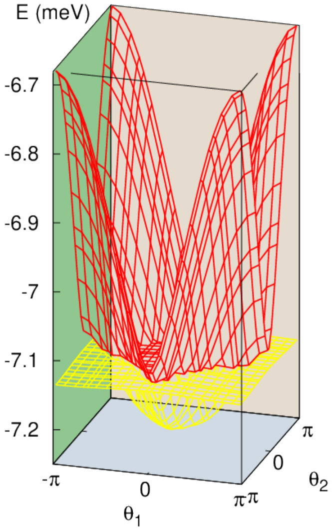
$N_e = 8$

red line ∼ 0 photon

yellow line ∼ 1 photons

The first photon replica of the lowest state is narrow at $g^{EM} = 0.01$, but at $g^{EM} = 0.10$ it has changed into a broad band that "interactcs" with a band just above the chemical potential and creates a kind of a splitting with an exchange of photon content, but now in two-dimensions in $\bar{\Theta}$-space

Rabi-resonances → variable anticrossing over the whole Brillouin zone



Summary

- Exact diagonalization $\leftrightarrow$ small systems
- Open systems $\leftrightarrow$ transport, high-order single-mode QED
- Large 2DEG $\leftrightarrow$ QEDFT (GGA), many γ-modes
- e-γ influence on magnetization, total energy
- Real-time excitations $\leftrightarrow$ red-shift of collective oscillations
- QED-DFT-TP

- Andrei Manolescu (RU)
- Valeriu Moldoveanu (NIMP)
- Nzar Rauf Abdullah (US)
- Chi-Shung Tang (NUU)
- Vram Mughnetsyan (YSU)
- Hsi-Sheng Goan (NTU)
- Jeng-Da Chai (NTU)

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

Appendix QED

$$H = \int d\boldsymbol{r}\ \psi^\dagger(\mathbf{r}) \left\{ \frac{\pi^2}{2m^*} + V(\mathbf{r}) \right\} \psi(\mathbf{r})$$

$$+ H_{\mathrm{EM}} + H_{\mathrm{Coul}} + H_{\mathrm{Z}}$$

$$+ \frac{1}{c} \int d\boldsymbol{r}\ \mathbf{j}(\mathbf{r}) \cdot \mathbf{A}_\gamma + \frac{e^2}{2m^* c^2} \int d\boldsymbol{r}\ n_e(\mathbf{r}) A_\gamma^2$$

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

with

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

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

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Appendix DFT - LSDA

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

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

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

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

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

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

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

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

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

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V. Gudmundsson, C.-S. Tang, and A. Manolescu, *Phys. Rev. B* **68**, 165343 (2003)
M. Koskinen, M. Manninen, and S. M. Reimann, *Phys. Rev. Lett.* **79**, 1389 (1997)

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Appendix AC-FDT

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

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

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

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

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

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

...

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

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

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

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