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Ab initio quantum electrodynamics: from bare masses to modifications of thermodynamics

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Foundations and Extensions of Density-Functional Theory

2 December, OsloMet Quantum Hub 2024

Outline

Interactions

- Light-matter interactions in quantum electrodynamics

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- Transverse and longitudinal photon modes

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Non-relativistic quantum electrodynamics (NRQED)

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- Pauli-Fierz Hamiltonian

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- Long-wavelength approximation

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Conclusion and outlook

Light-matter interactions: the origin of (most) matter properties

Photons: mediating the interactions between charged particles

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Gauge coupling (local charge conservation)

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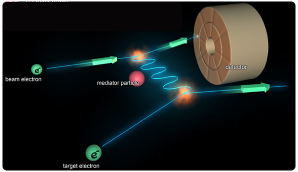

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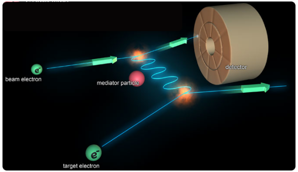

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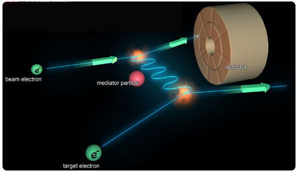

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Photon modes: transverse and longitudinal contributions

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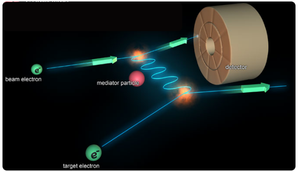

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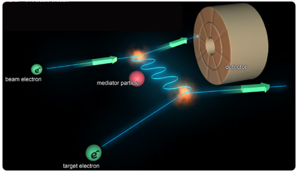

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Photon modes: transverse and longitudinal contributions

$$\underbrace{\left(\nabla\times\nabla\times - \nabla\nabla\cdot\right)}_{=-\nabla^2}\boldsymbol{f}_{\boldsymbol{k},\lambda}(\boldsymbol{r}) = \boldsymbol{k}^2\boldsymbol{f}_{\boldsymbol{k},\lambda}(\boldsymbol{r}) \qquad \boldsymbol{f}_{\boldsymbol{k},\lambda}(\boldsymbol{r}) = \epsilon(\boldsymbol{k},\lambda)\frac{\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})}{(2\pi)^{3/2}}$$

$$\boldsymbol{k}\cdot\epsilon(\boldsymbol{k},1) = \boldsymbol{k}\cdot\epsilon(\boldsymbol{k},2) = 0$$

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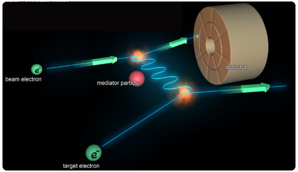

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Choosing a representation of light: Coulomb gauge

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$$\frac{1}{c}\int \hat{J}_\mu(x)\hat{A}^\mu(x)dx \rightarrow -\frac{1}{c}\int \hat{\boldsymbol{J}}(\boldsymbol{r})\cdot\hat{\boldsymbol{A}}_\perp(\boldsymbol{r})d\boldsymbol{r} + e^2\sum_\sigma \int\int \frac{\hat{\Psi}^\dagger(\boldsymbol{r}\sigma)\hat{\Psi}^\dagger(\boldsymbol{r}'\sigma)\hat{\Psi}(\boldsymbol{r}'\sigma)\hat{\Psi}(\boldsymbol{r}\sigma)}{4\pi\epsilon_0|\boldsymbol{r}-\boldsymbol{r}'|}d\boldsymbol{r}d\boldsymbol{r}'$$

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$$\hat{\boldsymbol{A}}_\perp(\boldsymbol{r}) = \sqrt{\frac{\hbar c^2}{\epsilon_0(2\pi)^3}}\sum_\lambda \int \frac{\boldsymbol{\epsilon}(\boldsymbol{k},\lambda)}{\sqrt{2\omega_{\boldsymbol{k}}}}\left(\hat{a}(\boldsymbol{k},\lambda)\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) + \hat{a}^\dagger(\boldsymbol{k},\lambda)\exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})\right)d\boldsymbol{k}$$

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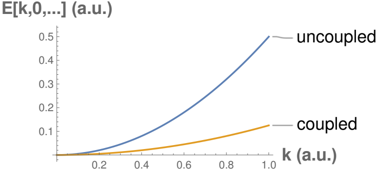

V.Rokaj PRR 013012 (2022)

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3D free space $\alpha \equiv (\boldsymbol{k},\lambda)$

$$\frac{\hbar^2}{2m}\left[\boldsymbol{k}^2 - \sum_\alpha \frac{\omega_{\mathrm{d}}^2}{\tilde{\omega}_\alpha^2}(\tilde{\epsilon}_\alpha\cdot\boldsymbol{k})^2\right] + \sum_\alpha \hbar\tilde{\omega}_\alpha\tilde{n}_\alpha$$

$$m_{\mathrm{ren}} = m\left(1 - \frac{4\alpha_{\mathrm{fs}}}{3\pi}\frac{\hbar\Lambda}{mc}\right)^{-1} \approx m + \frac{4\alpha_{\mathrm{fs}}}{3\pi}\frac{\hbar\Lambda}{c}$$

Modifying matter properties: changing light-matter interactions

Changing mode structure and coupling strength: photonic structures

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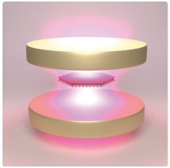
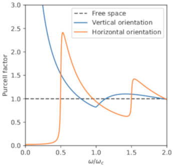
Changing mode structure and coupling strength: photonic structures





M.Svendsen arXiv:2312.17374

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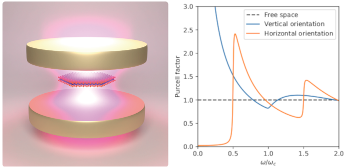

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Modes $(\tilde{\epsilon}_\alpha, \omega_\alpha) \Rightarrow m_{\mathrm{ren}}$ and $\hat{W}$ change

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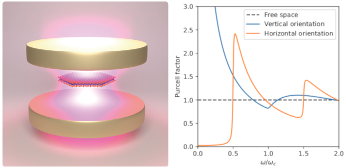

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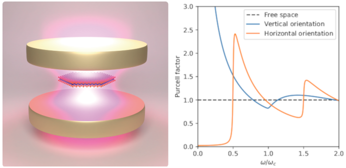

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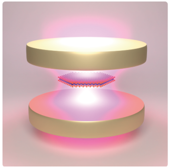

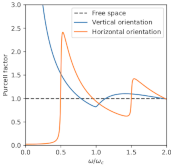

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$$\frac{\hbar^2}{2m}\left[\sum_l \boldsymbol{k}_l^2 - \sum_\alpha \frac{\omega_{\text{d}}^2}{N\tilde{\omega}_\alpha^2}\left(\tilde{\epsilon}_\alpha \cdot \sum_l \boldsymbol{k}_l\right)^2\right] + \sum_\alpha \hbar\tilde{\omega}_\alpha \tilde{n}_\alpha$$

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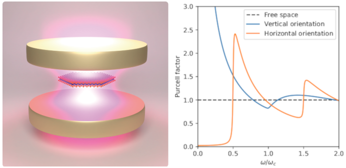

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Make one l distinguishable

$$\frac{\hbar^2}{2m}\left[\sum_l \boldsymbol{k}_l^2 - \sum_\alpha \frac{\omega_{\text{d}}^2}{N\tilde{\omega}_\alpha^2}\left(\tilde{\epsilon}_\alpha \cdot \sum_l \boldsymbol{k}_l\right)^2\right] + \sum_\alpha \hbar\tilde{\omega}_\alpha \tilde{n}_\alpha$$

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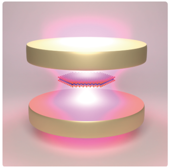

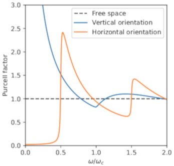

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$$\frac{\hbar^2}{2m}\left[\sum_l \boldsymbol{k}_l^2 - \sum_\alpha \frac{\omega_{\mathrm{d}}^2}{N\tilde{\omega}_\alpha^2}\left(\tilde{\epsilon}_\alpha \cdot \sum_l \boldsymbol{k}_l\right)^2\right] + \sum_\alpha \hbar\tilde{\omega}_\alpha \tilde{n}_\alpha \Rightarrow \frac{\hbar^2}{2m}\left[\boldsymbol{k}^2 - \sum_\alpha \frac{\omega_{\mathrm{d}}^2\left(\sum_{m\neq l}\tilde{\epsilon}_\alpha \cdot \boldsymbol{k}_m\right)^2}{\tilde{\omega}_\alpha^2 N}\left(\tilde{\epsilon}_\alpha \cdot \boldsymbol{k}\right)^2\right]$$

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Collective coupling: more is different

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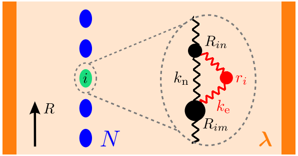

J.Horak arXiv:2401.16374

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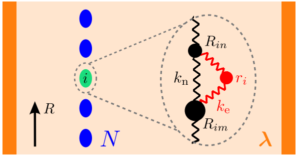

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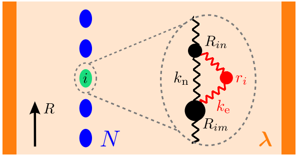
Free space $\alpha_i \Rightarrow \alpha = N\alpha_i$

Modifying matter properties: changing light-matter interactions

Collective coupling: more is different



J.Horak arXiv:2401.16374

Free space $\alpha_i \Rightarrow \alpha = N\alpha_i$

$$\tilde{\alpha}_i = \alpha_i \gamma^2(1, g), \ldots, \tilde{\alpha} = (N\alpha_i)\gamma^2(N, g)$$

$$\gamma^2(N, g) = \frac{1}{1+g^2 N\alpha_i},$$

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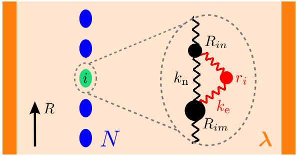

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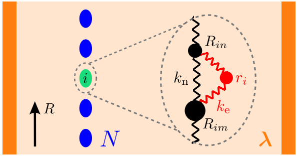

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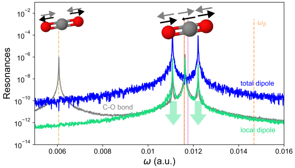

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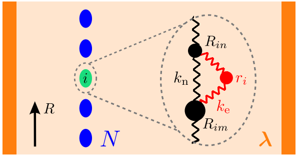

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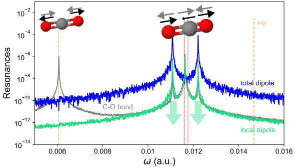

Experimental demonstrations with optical cavities

Modifying matter properties: changing light-matter interactions

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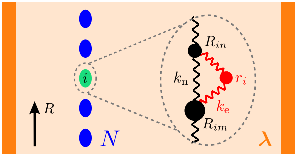

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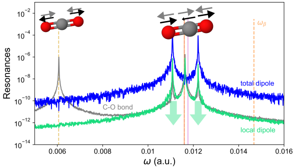

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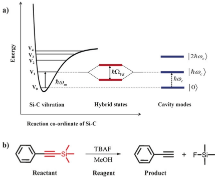

A.Thomas Ang.Chem.2016

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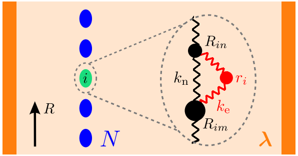

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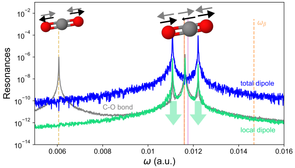

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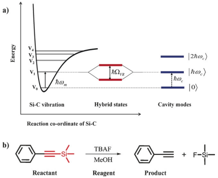

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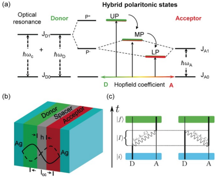

X.Zhong Ang.Chem.2019

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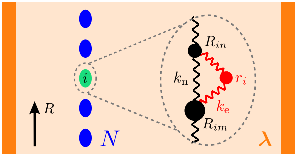

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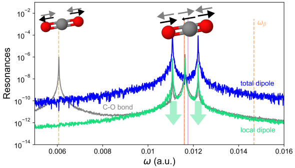

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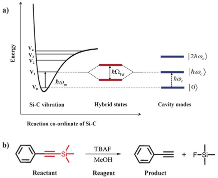

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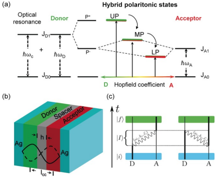

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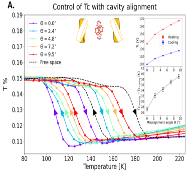

G.Jarc Nature 2023

First principles: non-relativistic (for matter) quantum electrodynamics

First principles: non-relativistic (for matter) quantum electrodynamics

mpsd

$$
\begin{aligned}
\hat{H}_{\mathrm{PF}} = &\sum_{l=1}^{N_e} \frac{1}{2m} \left[\left(-i\hbar\boldsymbol{\nabla}_{\boldsymbol{r}_l} + \frac{|e|}{c}\hat{\boldsymbol{A}}_{\perp}(\boldsymbol{r}_l)\right)\right]^2 + \frac{|e|\hbar}{2m}\boldsymbol{\sigma}_l \cdot \hat{\boldsymbol{B}}(\boldsymbol{r}_l) + \frac{1}{2}\sum_{l \neq m}^{N_e} \frac{e^2}{4\pi\epsilon_0 |\boldsymbol{r}_l - \boldsymbol{r}_m|} \\
&+ \sum_{l=1}^{N_n} \frac{1}{2M_l} \left[\left(-i\hbar\boldsymbol{\nabla}_{\boldsymbol{R}_l} - \frac{Z_l|e|}{c}\hat{\boldsymbol{A}}_{\perp}(\boldsymbol{R}_l)\right)\right]^2 - \frac{Z_l|e|\hbar}{2M_l}\boldsymbol{S}_l \cdot \hat{\boldsymbol{B}}(\boldsymbol{R}_l) + \frac{1}{2}\sum_{l \neq m}^{N_n} \frac{Z_l Z_m e^2}{4\pi\epsilon_0 |\boldsymbol{R}_l - \boldsymbol{R}_m|} \\
&- \sum_{l}^{N_e}\sum_{m}^{N_n} \frac{Z_m e^2}{4\pi\epsilon_0 |\boldsymbol{r}_l - \boldsymbol{R}_m|} + \sum_{\lambda=1}^{2} \int \mathrm{d}^3 k\, \hbar\omega_k \hat{a}^{\dagger}(\lambda, \boldsymbol{k})\hat{a}(\lambda, \boldsymbol{k}),
\end{aligned}
$$

H.Spohn, *Dynamics of Charged Particles and their Radiation Field*, Cambridge University Press (2004).

First principles: non-relativistic (for matter) quantum electrodynamics

mpsd

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$$+ \sum_{l=1}^{N_n}\frac{1}{2M_l}\left[\left(-i\hbar\boldsymbol{\nabla}_{\boldsymbol{R}_l} - \frac{Z_l|e|}{c}\hat{\boldsymbol{A}}_{\perp}(\boldsymbol{R}_l)\right)\right]^2 - \frac{Z_l|e|\hbar}{2M_l}\boldsymbol{S}_l\cdot\hat{\boldsymbol{B}}(\boldsymbol{R}_l) + \frac{1}{2}\sum_{l\neq m}^{N_n}\frac{Z_l Z_m e^2}{4\pi\epsilon_0|\boldsymbol{R}_l - \boldsymbol{R}_m|}$$
$$- \sum_{l}^{N_e}\sum_{m}^{N_n}\frac{Z_m e^2}{4\pi\epsilon_0|\boldsymbol{r}_l - \boldsymbol{R}_m|} + \sum_{\lambda=1}^{2}\int \mathrm{d}^3k\,\hbar\omega_k\,\hat{a}^{\dagger}(\lambda,\boldsymbol{k})\hat{a}(\lambda,\boldsymbol{k}),$$

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First principles: non-relativistic (for matter) quantum electrodynamics

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$$-\sum_{l}^{N_e}\sum_{m}^{N_n}\frac{Z_me^2}{4\pi\epsilon_0|\boldsymbol{r}_l-\boldsymbol{R}_m|} + \sum_{\lambda=1}^{2}\int \mathrm{d}^3k\,\hbar\omega_k\,\hat{a}^{\dagger}(\lambda,\boldsymbol{k})\hat{a}(\lambda,\boldsymbol{k}),$$

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First principles: non-relativistic (for matter) quantum electrodynamics

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$$-\sum_{l}^{N_e}\sum_{m}^{N_n}\frac{Z_m e^2}{4\pi\epsilon_0|\boldsymbol{r}_l-\boldsymbol{R}_m|} + \sum_{\lambda=1}^{2}\int \mathrm{d}^3k\,\hbar\omega_k\,\hat{a}^{\dagger}(\lambda,\boldsymbol{k})\hat{a}(\lambda,\boldsymbol{k}),$$

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− Ultra-violet regularization (question of non-perturbative renormalizability)

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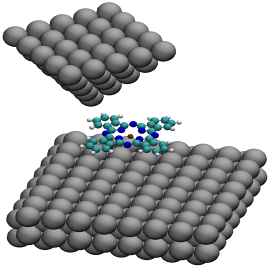
From full to approximate first-principles



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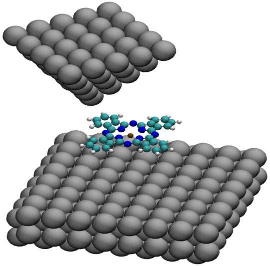
From full to approximate first-principles



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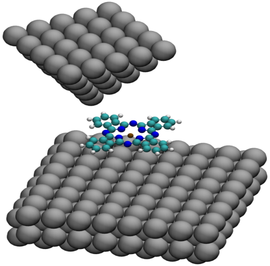
Long-wavelength approximation

1. Wavelengths/modes $\gg$ system size

From full to approximate first-principles



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Long-wavelength approximation

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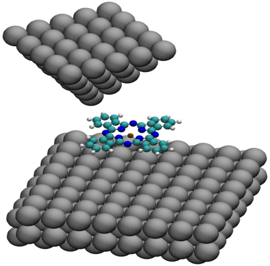
From full to approximate first-principles

mpsd



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$$\hat{H}'_{\mathrm{PF}} = \underbrace{\sum_{i=1}^{N} -\frac{\hbar^2}{2m_i}\nabla_i^2 + \sum_{i>j}^{N} w(\boldsymbol{r}_i, \boldsymbol{r}_j)}_{\text{electron-ion}} + \underbrace{\frac{\hbar^2}{2}\sum_{\alpha}\Big[-\frac{\partial^2}{\partial p_\alpha^2} + \omega_\alpha^2\Big(p_\alpha + \frac{g_\alpha \epsilon_\alpha}{\omega_\alpha}\cdot \overbrace{\sum_{i=1}^{N} Z_i |e| \boldsymbol{r}_i}^{=\hat{\boldsymbol{R}}}\Big)^2\Big]}_{\text{photonic+dipole coupling}}$$

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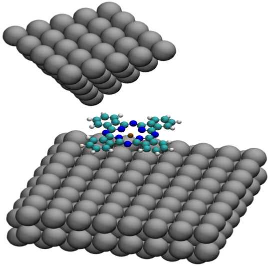

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- $(g_\alpha, \epsilon_\alpha, \omega_\alpha)$ from, e.g., MQED

M.Svendsen etal., JCTC 20, 926-936 (2024).

From full to approximate first-principles

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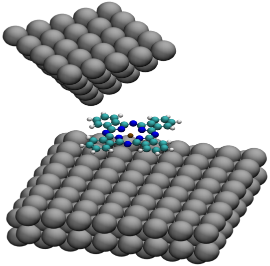

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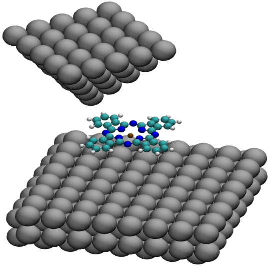

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- $\hat{\mathbf{R}}^2$ necessary

M.Svendsen etal., JCTC **20**, 926-936 (2024). V.Rokaj etal., J. Phys. B **51**, 034005 (2018), C.Schäfer etal., ACS photonics **7**, 975 (2020).

Playground for quantum many-body methods

Exponential wall for wave functions

Already small systems with only few effective modes need HPC

Record: three (quantum mechanical) particles plus one mode

D. Sidler etal., J. Phys. Chem. Lett. 11, 7525 (2020); JCTC 19, 8801-8814 (2024)

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MR etal., Phys. Rev. A 90, 012508 (2014); MR, arXiv:1509.01417 (2015); R.Jestädt etal., Adv. Phys. 68, 225 (2019).

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$$\vdots$$

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$$\vdots$$

Discarding transverse modes leads to standard ground-state mapping: $v_{\mathrm{ext}}(\boldsymbol{r}) \leftrightarrow \rho(\boldsymbol{r})$

MR etal., Phys. Rev. A 90, 012508 (2014); MR, arXiv:1509.01417 (2015); R.Jestädt etal., Adv. Phys. 68, 225 (2019).

Conclusion and Outlook

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- Light-matter interactions from first principles:

Conclusion and Outlook

Conclusion

- Light-matter interactions from first principles:
  - Bare vs. renormalized/observable masses

Conclusion and Outlook

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- Quantum-electrodynamical density-functional theories (QEDFT)

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mpsd

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Thank you for your attention!

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