Quantum-Electrodynamical Density-Functional Theory

for the Quantum Rabi Model

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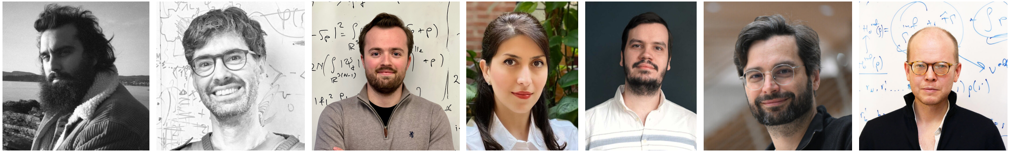
Acknowledgements

Collaboration with M. A. Csirik,[1,2] M. Penz,[1,3] V. Bakkestuen,[1] M. Lotfigolian[1], A. Davidov[1], M. Ruggenthaler,[3] and A. Laestadius.[1,2]



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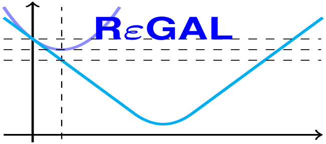

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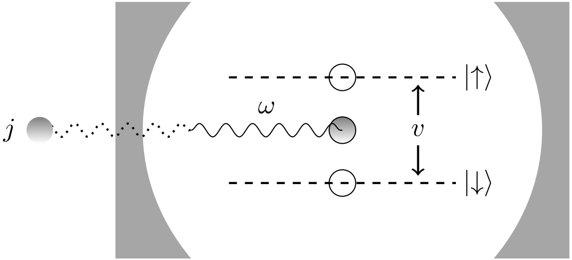
Motivation and Introduction

- Light-matter interactions
- Ground-state effects of photon-electron coupling
- This talk: The Quantum Rabi model [1].
  - One of the simplest models one can study
  - (Almost) explicit form of a DFT functional
- Later today: The (multi-mode) Dicke model [2].

The Quantum Rabi Model

$$\hat{H}_0 = \underbrace{\frac{1}{2}\hat{p}^2 + \frac{\omega^2}{2}\hat{x}^2}_{\text{QHO}} - \overbrace{t\hat{\sigma}_x}^{\text{TLS kin.}} + \underbrace{g\hat{\sigma}_z\hat{x}}_{\text{TLS QHO coupling}}$$

$$\hat{H}(v, j) = \hat{H}_0 + v\hat{\sigma}_z + j\hat{x}$$



$$\psi(x) = \begin{pmatrix} \psi_+(x) \\ \psi_-(x) \end{pmatrix} \in L^2(\mathbb{R}, \mathbb{C}^2)$$

$$\|\psi\|^2 = \|\psi_+\|_{L^2}^2 + \|\psi_-\|_{L^2}^2 = 1$$

Ground state:

- Unique
- Real
- Strictly positive

Densities and potentials

We define two “densities”:

$$\sigma_\psi = \langle \widehat{\sigma}_z \rangle_\psi \in [-1, 1]$$
$$\xi_\psi = \langle \widehat{x} \rangle_\psi \in \mathbb{R}$$

	DFT	QEDFT Q. Rabi
Dens.	ρ	(σ, ξ)
Pot.	v	(v, j)
N-rep.	I_N	$[-1, 1] \times \mathbb{R}$
v-rep.	?	$(-1, 1) \times \mathbb{R}$

Energy and Functionals

Variational formulation

$$E(v,j) = \min_{\psi} \langle \widehat{H}(v,j) \rangle_\psi$$
$$= \min_{\sigma,\xi} \{ F_{\mathrm{LL}}(\sigma,\xi) + v\sigma + j\xi \}$$
$$F_{\mathrm{LL}}(\sigma,\xi) = \min_{\psi \mapsto (\sigma,\xi)} \langle \widehat{H}_0 \rangle_\psi$$

The dependence on ξ is explicitly

$$F_{\mathrm{LL}}(\sigma,\xi) = F_{\mathrm{LL}}(\sigma,0) + g\sigma\xi + \frac{\omega^2}{2}\xi^2$$

The optimiser of F_{LL} is the ground state of $\widehat{H}(v,j)$:

$$F_{\mathrm{LL}}(\sigma,\xi) = F_{\mathrm{L}}(\sigma,\xi)$$
$$= \max_{v,j} \{ E(v,j) - v\sigma - j\xi \}$$

Consequences for F_{LL}:

- Convex
- Differentiable

Potentials From Differentiation

Recall

$$E(v,j) = \min_{\sigma,\xi}\{F_{\mathrm{LL}}(\sigma,\xi) + v\sigma + j\xi\}$$

$$F_{\mathrm{LL}}(\sigma,\xi) = F_{\mathrm{LL}}(\sigma,0) + g\sigma\xi + \frac{\omega^2}{2}\xi^2$$

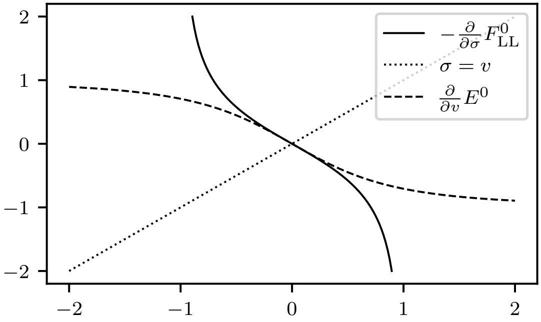
Then

$$-v = \frac{\partial F_{\mathrm{LL}}}{\partial \sigma}, \quad -j = \frac{\partial F_{\mathrm{LL}}}{\partial \xi} = g\sigma + \omega^2\xi$$

In standard DFT, $-v \in \underline{\partial} F_{\mathrm{L}}(\rho)$.

F_{LL} and E contain the same information:

$$-(v,j) \in \underline{\partial} F_{\mathrm{LL}}(\sigma,\xi) \iff (\sigma,\xi) \in \overline{\partial} E(v,j)$$



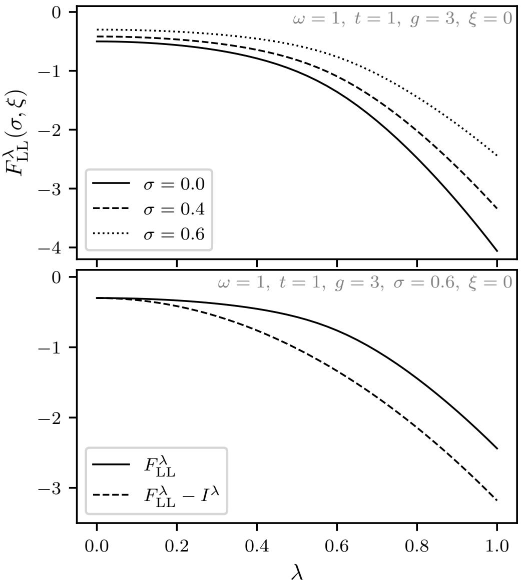
Adiabatic connection

$$\hat{H}_0^\lambda = \frac{1}{2}\hat{p}^2 + \frac{\omega^2}{2}\hat{x}^2 - t\hat{\sigma}_x + \lambda g\hat{\sigma}_z\hat{x}$$

Functional is concave in λ:

$$\begin{aligned} F_{\mathrm{LL}}^\lambda(\sigma,0) =& F_{\mathrm{LL}}^0(\sigma,0) + \int_0^\lambda f^\nu(\sigma)\mathrm{d}\nu, \\ f^\nu(\sigma) =& g\langle\hat{\sigma}_z\hat{x}\rangle_{\varphi^\nu(\sigma)}, \end{aligned}$$

where φ^ν is the optimiser of $F_{\mathrm{LL}}^\nu(\sigma,0)$.



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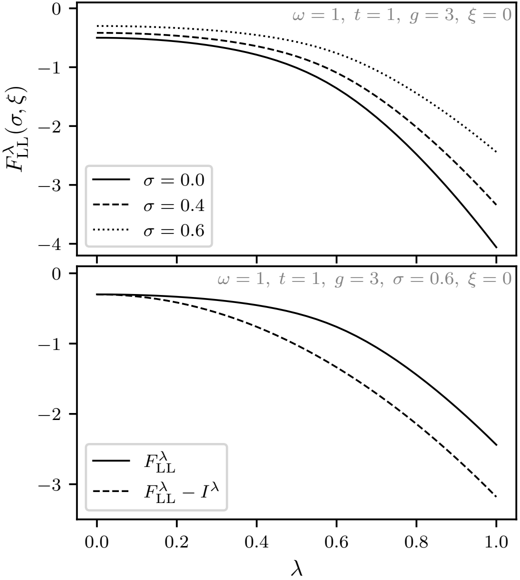
Almost explicit form

$$F_{\mathrm{LL}}^{\lambda}(\sigma,\xi) = \frac{\omega}{2} - t\sqrt{1-\sigma^2} + \frac{\omega^2}{2}\xi^2 + \lambda g \sigma \xi - \frac{\lambda^2 g^2}{2\omega^2} + I^{\lambda}(\sigma),$$

$$I^{\lambda}(\sigma) = -\frac{4tg}{\omega^2}\int_0^{\lambda}\int \varphi_+^{\nu\,\prime}\varphi_-^{\nu}\,\mathrm{d}x\mathrm{d}\nu,$$



Approximation to the non-explicit term

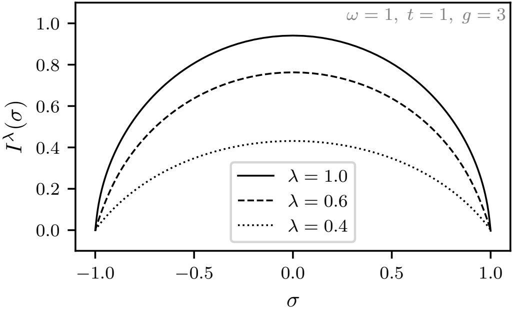
Bounds

- $I^\lambda(\sigma) \geq 0$
- $I^\lambda(\sigma) \leq \frac{\lambda^2 g^2}{2\omega^2}(1-\sigma^2)$
- $I^\lambda(\sigma) \leq t\sqrt{1-\sigma^2}\left(1 - \exp\left\{-\frac{\lambda^2 g^2}{\omega^3}\right\}\right)$

Approximate form

$$I^\lambda(\sigma) \approx b\left(\sqrt{1-\frac{\sigma^2}{a^2}} - \sqrt{1-\frac{1}{a^2}}\right)$$

with new parameters a and b which depend on t and λ.



Bounds

- $I^\lambda(\sigma) \geq 0$
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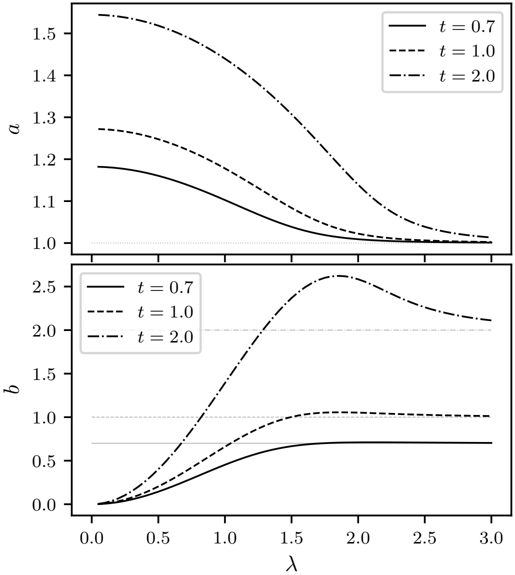
- $I^\lambda(\sigma) \leq t\sqrt{1-\sigma^2}\left(1-\exp\left\{-\frac{\lambda^2 g^2}{\omega^3}\right\}\right)$

Approximate form

$$I^\lambda(\sigma) \approx b\left(\sqrt{1-\frac{\sigma^2}{a^2}}-\sqrt{1-\frac{1}{a^2}}\right)$$

- $\lim_{\lambda\to\infty} a = 1$
- $\lim_{\lambda\to 0} b = 0$
- $\lim_{\lambda\to\infty} b = t$



Conclusions

- Illustrative example of QEDFT
- Its natural generalisations contain insights and challenges
- Explore further techniques in a controlled environment
  - Regularisation
  - Kohn–Sham
  - Inverse Kohn–Sham

References

1. **Bakkestuen, V. H., Falmår, V., Lotfigolian, M., Penz, M., Ruggenthaler, M. & Laestadius, A.** *Quantum-Electrodynamical Density-Functional Theory Exemplified by the Quantum Rabi Model.* 2024. arXiv: 2411.15256 [quant-ph]. https://arxiv.org/abs/2411.15256.
2. **Bakkestuen, V. H., Csirik, M. A., Laestadius, A. & Penz, M.** *Quantum-electrodynamical density-functional theory for the Dicke Hamiltonian.* 2024. arXiv: 2409.13767 [math-ph]. https://arxiv.org/abs/2409.13767.

Thank you for your attention!

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N-representability

For any $(\sigma, \xi) \in [-1, 1] \times \mathbb{R}$ there exists an admissable wavefunction ψ such that $\sigma_\psi = \sigma$ and $\xi_\psi = \xi$.

Proof by construction:

$$\psi(x) = \begin{pmatrix} c_+ \\ c_- \end{pmatrix} \sqrt[4]{\frac{\omega}{\pi}} e^{-\frac{\omega}{2}(x-\xi)^2}, \quad c_\pm = \sqrt{\frac{1 \pm \sigma}{2}}.$$