Ground and excited states of vibrationally dressed polaritons

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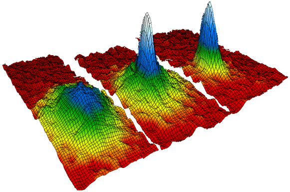
University of St Andrews
FOUNDED 1413

SUPA

SCOM, October 2016

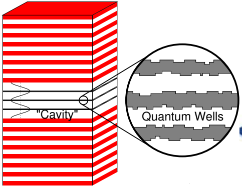
Condensation, Lasing, Superradiance

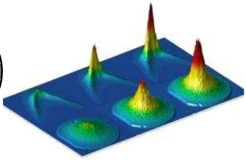
Atomic BEC $T \sim 10^{-7}$K



[Anderson *et al.* Science '95]

Polariton Condensate $T \sim 20$K

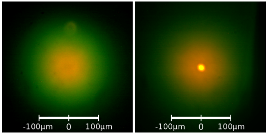




[Kasprzak *et al.* Nature, '06]

Photon Condensate

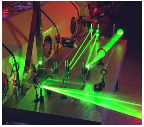
$T \sim 300$K



[Klaers *et al.* Nature, '10]

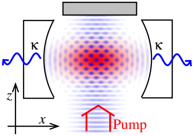
Laser

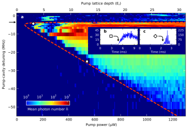
$T \sim ?, < 0, \infty$



Superradiance transition

$T \sim 0$





[Baumann *et al.* Nature '10]

Paradigms & Models

- Weakly interacting dilute Bose gas
  $$H = \int d^d r \hat{\psi}^\dagger(-\mu - \nabla^2)\hat{\psi} + U\hat{\psi}^\dagger\hat{\psi}^\dagger\hat{\psi}\hat{\psi}$$
  - Single field — assumes strong coupling
  - Continuum model, hard to include molecular physics
- Laser rate equations
  - Emission, absorption — assumes weak coupling, lasing.
- Complex Gross-Pitaevskii/Ginzburg Landau equations
  $$i\partial_t\psi = \left(-\nabla^2\psi + V(r) + U|\psi|^2\right)\psi + i\left(P(\psi, n, r) - \kappa\right)\psi$$
  - Applies to laser, condensate — fluids of light
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- Microscopic model . . .

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Simple models, *N* body physics

- Model capable of lasing & condensation
  - Tavis-Cummings / Dicke model

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  - High temperature: Maxwell-Bloch laser

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Szymanska et al. PRL 06; Keeling et al. book chapter 1010.3338

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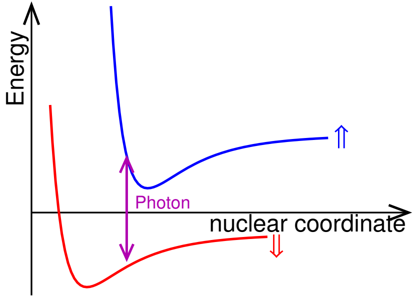

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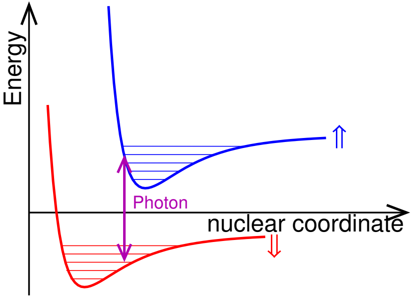

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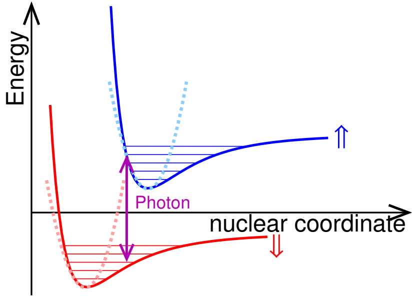

Holstein-Tavis-Cummings & Holstein-Dicke model

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Introduction and models

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   - Holstein-Dicke model
   - Weak coupling: photon BEC
2. Strong coupling: polariton states
   - Exact solutions
   - Scaling with N
3. Ultrastrong coupling: ground state changes

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HTC weak coupling

- Polaron transform (exact), $\mathcal{D}_i = e^{\lambda_0(\hat{b}_i^\dagger - \hat{b}_i)}$

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- Perturbation in g & dissipative processes

$$\dot{\rho} = -i[H_0, \rho] + \sum_m \frac{\kappa}{2}\mathcal{L}[\hat{a}_m] + \sum_i \left[\frac{\Gamma_\uparrow}{2}\mathcal{L}[\sigma_i^+] + \frac{\Gamma_\downarrow}{2}\mathcal{L}[\sigma_i^-] \right]$$

$$+ \sum_{m,i} \left[\frac{\Gamma(\delta_m = \omega_m - \omega_X)}{2}\mathcal{L}[\sigma_i^+ \hat{a}_m] + \frac{\Gamma(-\delta_m = \omega_X - \omega_m)}{2}\mathcal{L}[\sigma_i^- \hat{a}_m^\dagger] \right]$$

- Correlation function:

$$\Gamma(\delta) = 2g^2 \,\mathrm{Re}\left[\int dt e^{-i\delta t - (\Gamma_\uparrow + \Gamma_\downarrow)t/2} \langle D_i^\dagger(t) D_i(0) \rangle \right]$$

[Marthaler et al PRL '11, Kirton & JK PRL '13]

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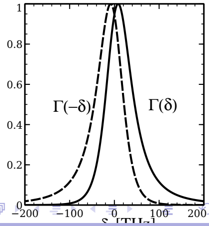

HTC weak-coupling and photon BEC

- Rate equation:

$$\partial_t n_m = -\kappa n_m + \Gamma(-\delta_m)(n_m + 1)\sum_i \langle \sigma_i^+ \sigma_i^- \rangle - \Gamma(\delta_m) n_m \sum_i \langle \sigma_i^- \sigma_i^+ \rangle$$

- Steady state distribution: $\frac{n_m}{n_m+1} = \frac{\Gamma(-\delta_m)\sum_i \langle \sigma_i^+ \sigma_i^- \rangle}{\Gamma(\delta_m)\sum_i \langle \sigma_i^- \sigma_i^+ \rangle}$
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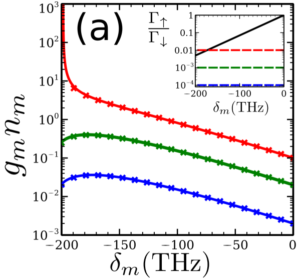

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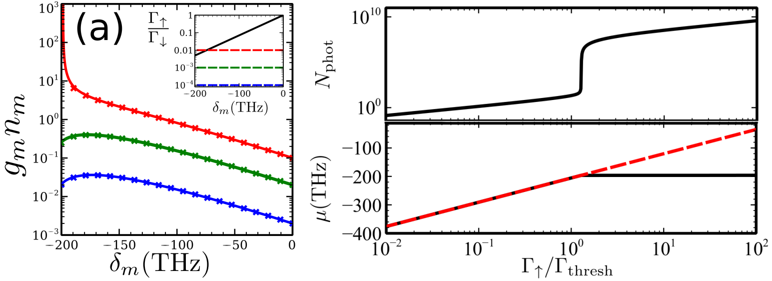

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Strong coupling: polariton states

One excitation subspace, questions

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- Rotating wave approximation — Holstein Tavis Cummings
- Restrict, $\hat{a}^\dagger \hat{a} + \sum_i \sigma_i^+ \sigma_i^- = 1$.
- Questions:
  - Competition of $g\sqrt{N}$ vs ω_v, $\omega_v \lambda_0^2$
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Exact solution, $N = 2$

Vibrational Wigner function:

$$W(x, p) = \int dy \langle x + y/2|\rho|x - y/2\rangle_i e^{iyp}, \quad \left(\frac{\hat{b}_i + \hat{b}_i^\dagger}{\sqrt{2}}\right)|x\rangle_i = x|x\rangle_i$$

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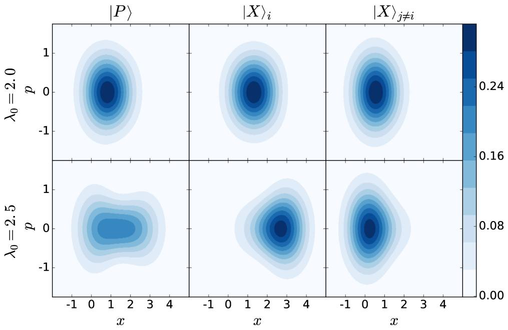
Conditioned on Photon $|P\rangle$/Exciton at i, $|X\rangle_i$/Other site $|X\rangle_{j \neq i}$



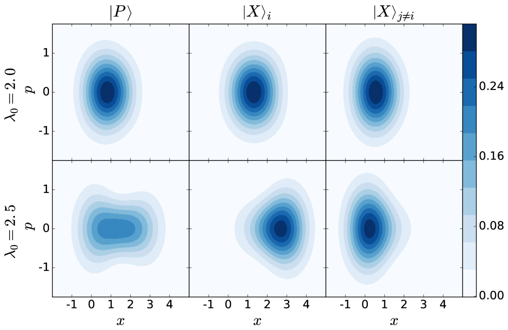
$N = 2, \omega = \omega_X, \omega_R \equiv g/\sqrt{N} = 1$

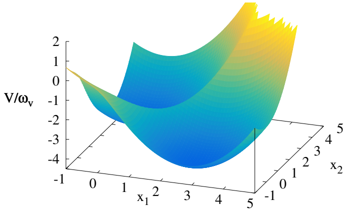
Exact solution, $N = 2$

Vibrational Wigner function:

$$W(x,p) = \int dy \langle x + y/2|\rho|x - y/2\rangle_i e^{iyp}, \quad \left(\frac{\hat{b}_i + \hat{b}_i^\dagger}{\sqrt{2}}\right)|x\rangle_i = x|x\rangle_i$$

Conditioned on Photon $|P\rangle$/Exciton at i, $|X\rangle_i$/Other site $|X\rangle_{j\neq i}$





$N = 2, \omega = \omega_X, \omega_R \equiv g/\sqrt{N} = 1$

Exact solution, larger N

- Brute force approach, N sites, $\hat{b}^\dagger \hat{b} < M$, $D_{\text{Hilbert}} = M^N$
- Permutation symmetry. $D_{\text{Hilbert}} \sim N^M$, typical $M \sim 5-6$

- Increasing N, suppress $W_{|P\rangle}(x \neq 0)$
- Distinct behaviour vs λ_0
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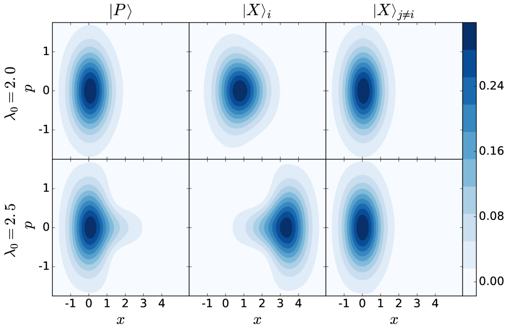

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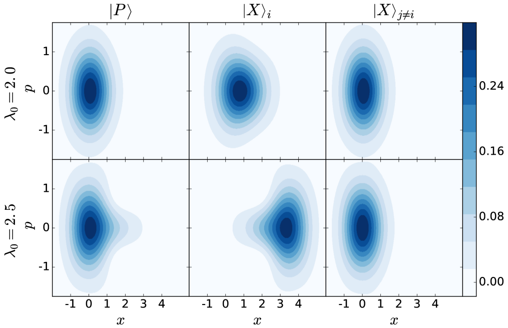

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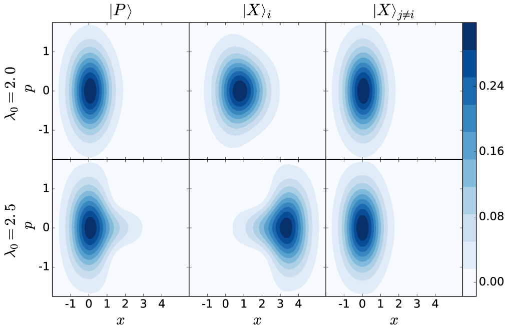

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Extending to arbitrary N, polaron ansatz

- Polaron transform, $\mathcal{D}_i(\lambda) = \exp\left(\lambda(\hat{b}_i^\dagger - \hat{b}_i)\right)$
- Single molecule ansatz:

$$|\Psi\rangle = [\alpha\mathcal{D}(\lambda_\uparrow)|\uparrow\rangle + \beta\mathcal{D}(\lambda_\downarrow)|\downarrow\rangle]|0\rangle_V$$

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$$|\Psi\rangle = \left[\alpha|P\rangle\prod_j \mathcal{D}_j(\lambda_a) + \frac{\beta}{\sqrt{N}}\sum_i |X\rangle_i \mathcal{D}_i(\lambda_b)\prod_{j\neq i}\mathcal{D}_j(\lambda_c)\right]|0\rangle_V$$

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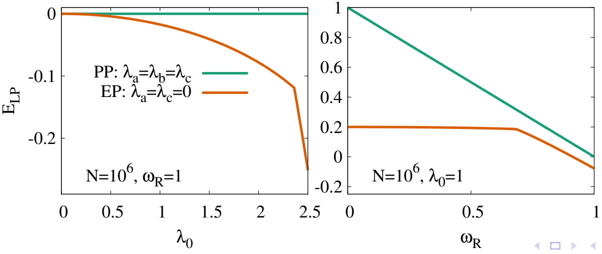

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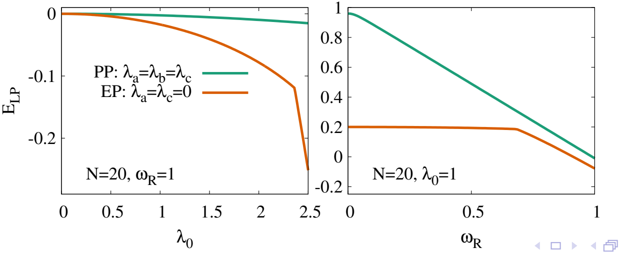

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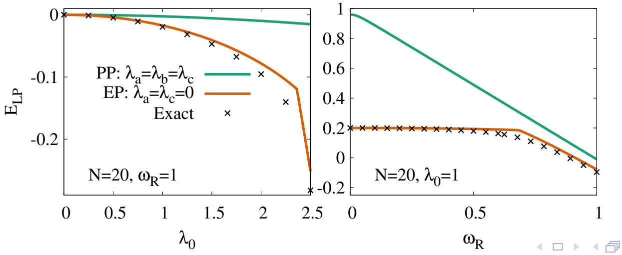
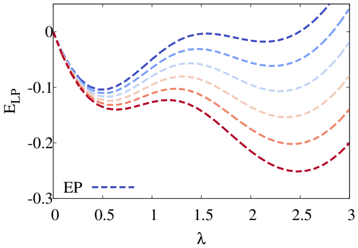


Polaron crossover

- Crossover near $\omega_R \simeq \omega_v \lambda_0^2$ [Silbey and Harris, J. Chem. Phys. 1984]



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  - Superpose multiple polarons
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- Simplifed 2-polaron form [Zeb *et al.* arXiv:1608.08929]

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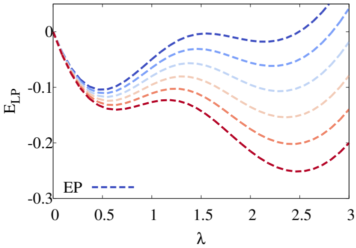

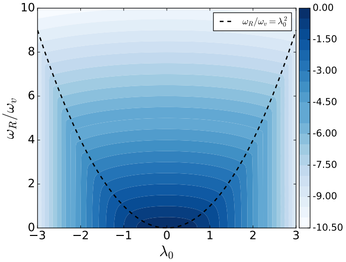

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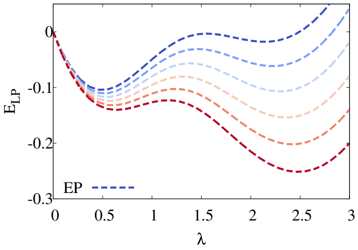

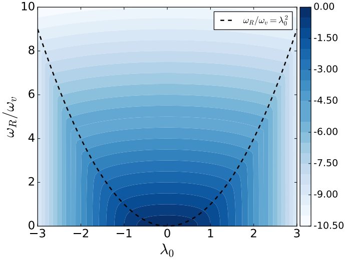

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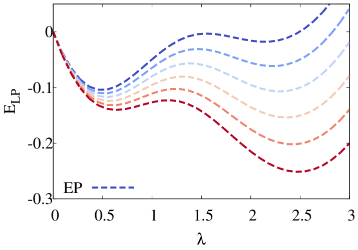

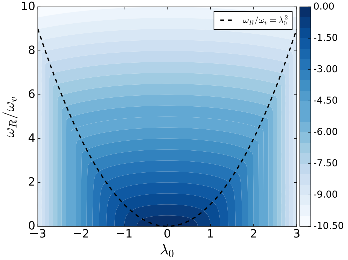

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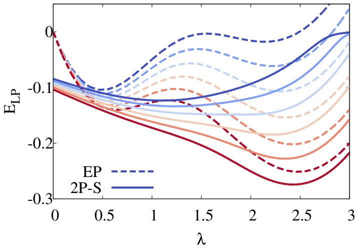

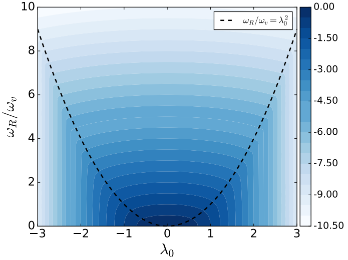

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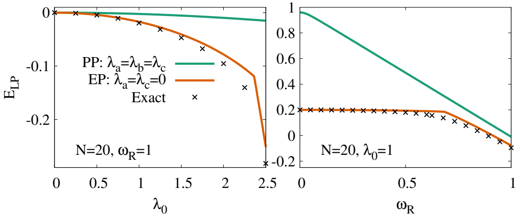
- Accurate energy & wavefunction



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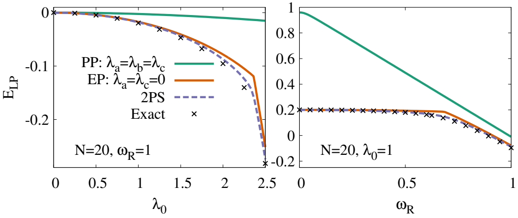

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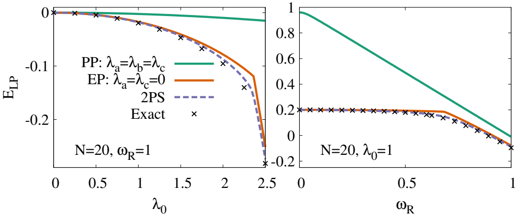

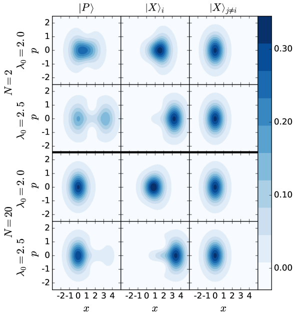

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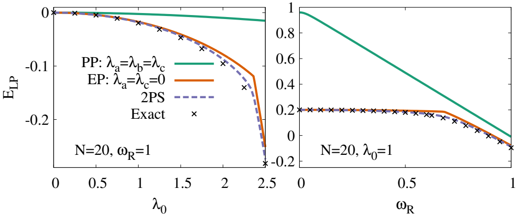

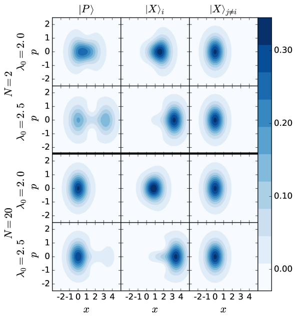

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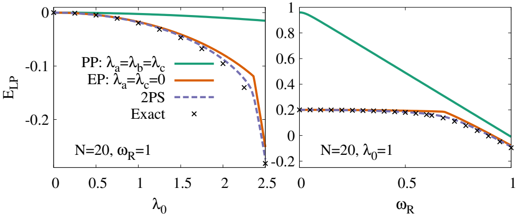

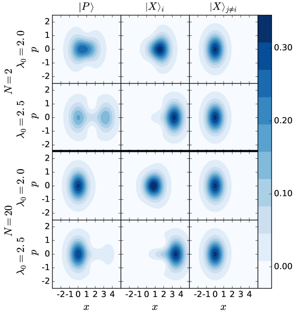

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Ultrastrong coupling: ground state changes

Ground state molecular reconfiguration

- Dicke model: beyond rotating wave approximation

$$H = \sum_K \omega_k \hat{a}_k^\dagger \hat{a}_k + \sum_{i=1}^{N} \left[\omega_X \sigma_i^+ \sigma_i^- + \sum_k g_{\mathbf{k}} \left(\sigma_i^+ (\hat{a}_k + \hat{a}_k^\dagger) + \text{H.c.} \right) + \dots \right]$$

- Effect on molecular structure?

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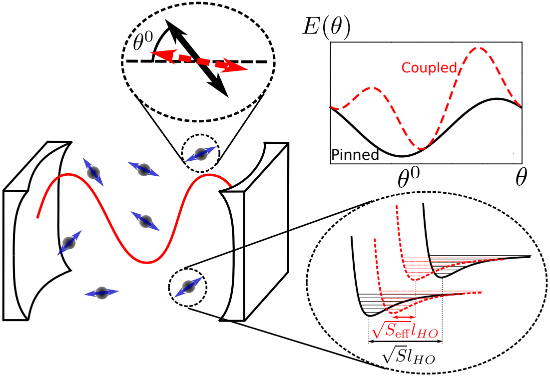
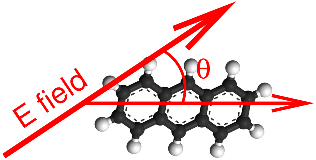


Rotational reorientation

- Rotational degrees of freedom



- Effective Hamiltonian

$$H = \ldots + \sum_{i,k}\left[\ldots + g_{i,\mathbf{k}}\cos(\theta_i)(\hat{a}^\dagger_{\mathbf{k}} + \hat{a}_{-\mathbf{k}})\sigma^x_i + E_0(\theta_i)\right]$$

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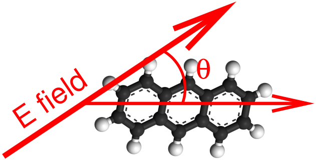

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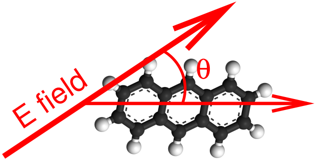

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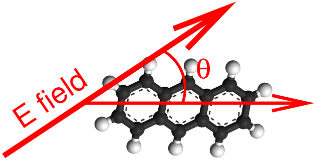

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Vibrational reconfiguration

- Schrieffer-Wolff – mixes vibrational states

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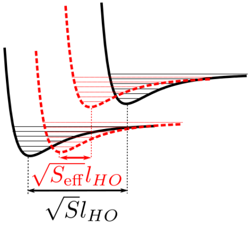

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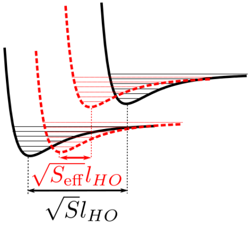

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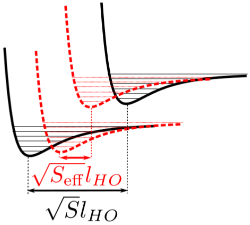

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Acknowledgements

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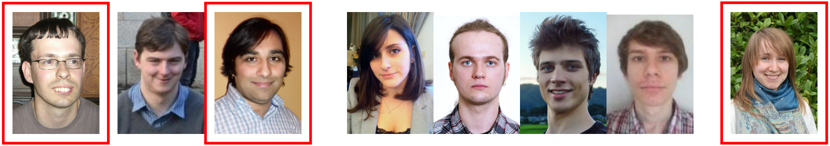

COLLABORATORS: S. De Liberato (Southhampton)

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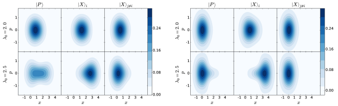
topnes
Topological Protection and Non-Equilibrium States in Strongly Correlated Electron Systems

Hybrid Polaritonics

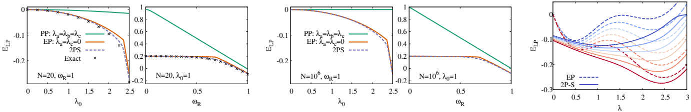
The Leverhulme Trust

Summary

- Holstein-Dicke and Holstein-Tavis-Cummings models
- Single polariton state
  - Exact solution

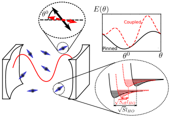


  - Polaron ansatz



[Zeb, Kirton, JK, `arXiv:1608.08929`]

- Ground state configuration



[Cwik, Kirton, De Liberato, JK, PRA 2016]