Recent surprises regarding polaron behavior in condensed matter systems

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Collaborators:

→ Glen Goodvin, Dominic Marchand, Lucian Covaci, Hadi Ebrahimnejad, Clemens Adolphs, Alfred Cheung, …

→ George Sawatzky and Philip Stamp

→ Holger Feshke, Andrey Mishchenko, Vittorio Cataudella, …

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Polaron = dressed quasiparticle

→ very old problem (Landau, 1933)

→ particle (electron, hole, exciton, …) interacts with bosons from its environment (phonons, magnons, orbitons, electron-hole pairs or plasmons, …)

→ particle is surrounded by a cloud of such excitations, that are continuously emitted and absorbed

→ renormalized properties because of the cloud – how strongly?

Today: a single particle → a single polaron in the system

→ think very weakly doped insulators, in condensed matter systems

→ ignore complications due to boson-mediated interactions between polarons, which can lead to superconductivity and all manner of other interesting properties

Very brief summary of the research from most of these past 80 years:

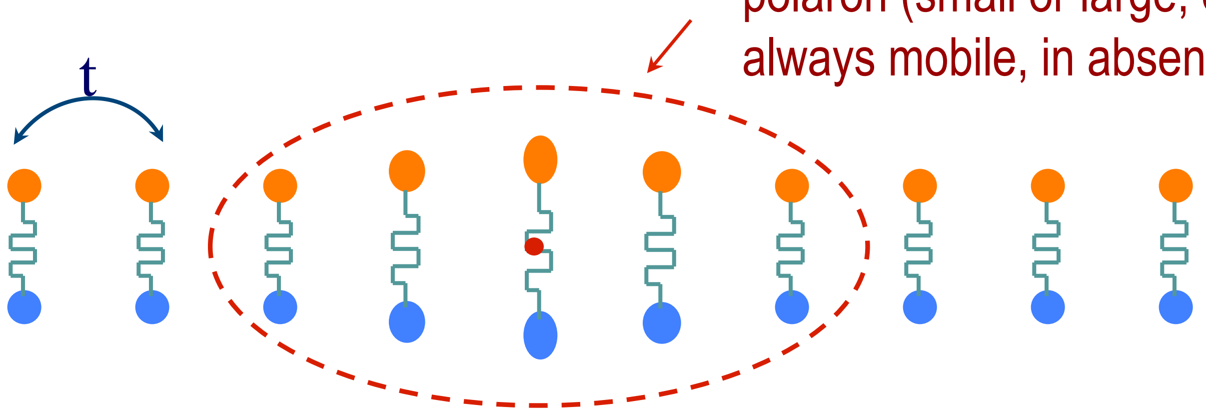
All models studied (Holstein, coupling to breathing-mode phonon, Frohlich, …) show qualitatively similar results …

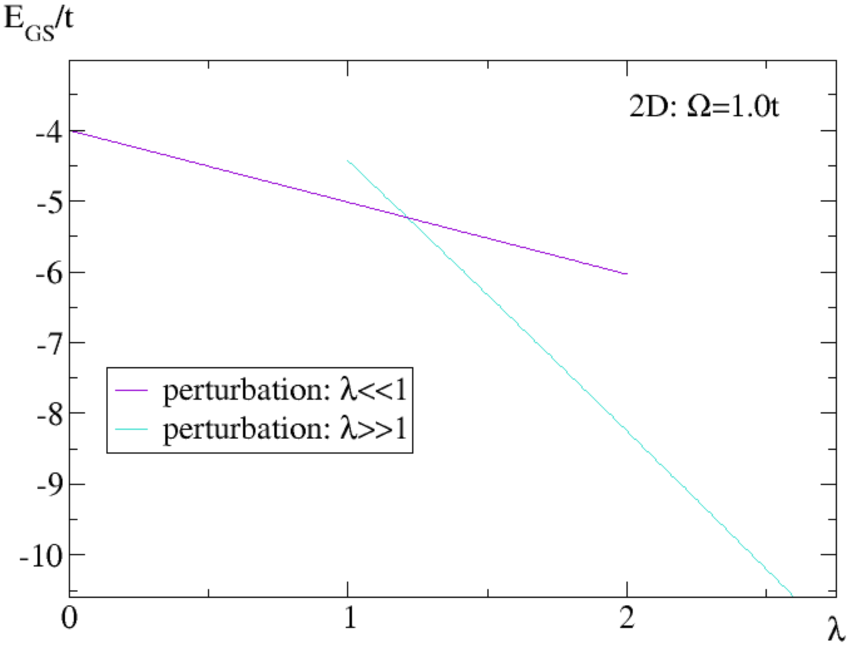
Holstein Hamiltonian = simplified description of a “molecular crystal”

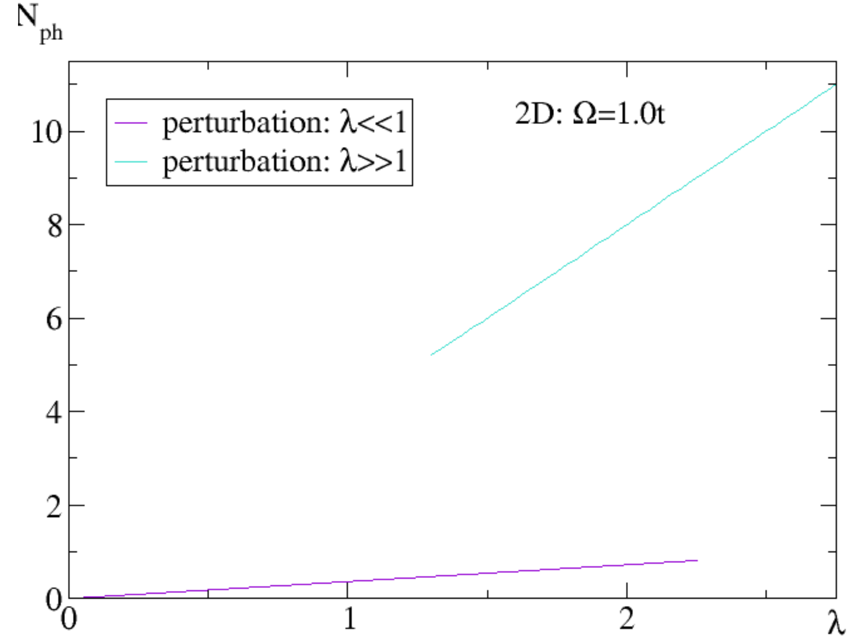
“unit cell” in equilibrium

= new equilibrium distance

polaron (small or large, depending) but always mobile, in absence of disorder

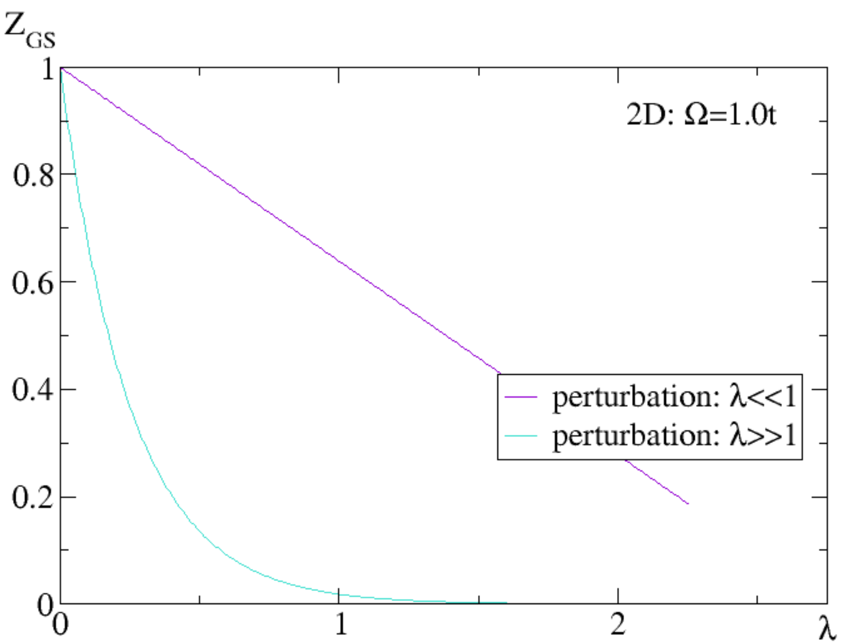


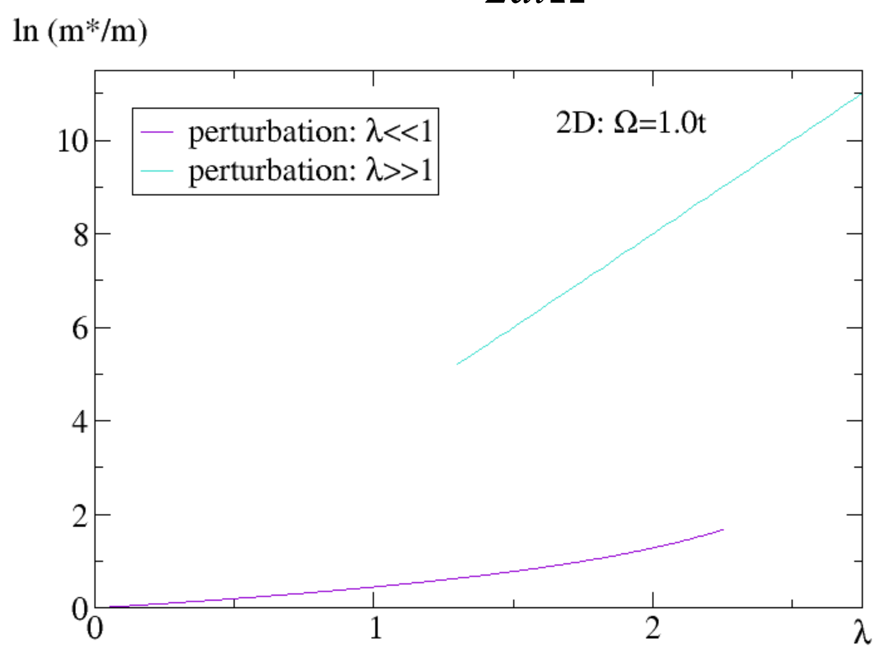


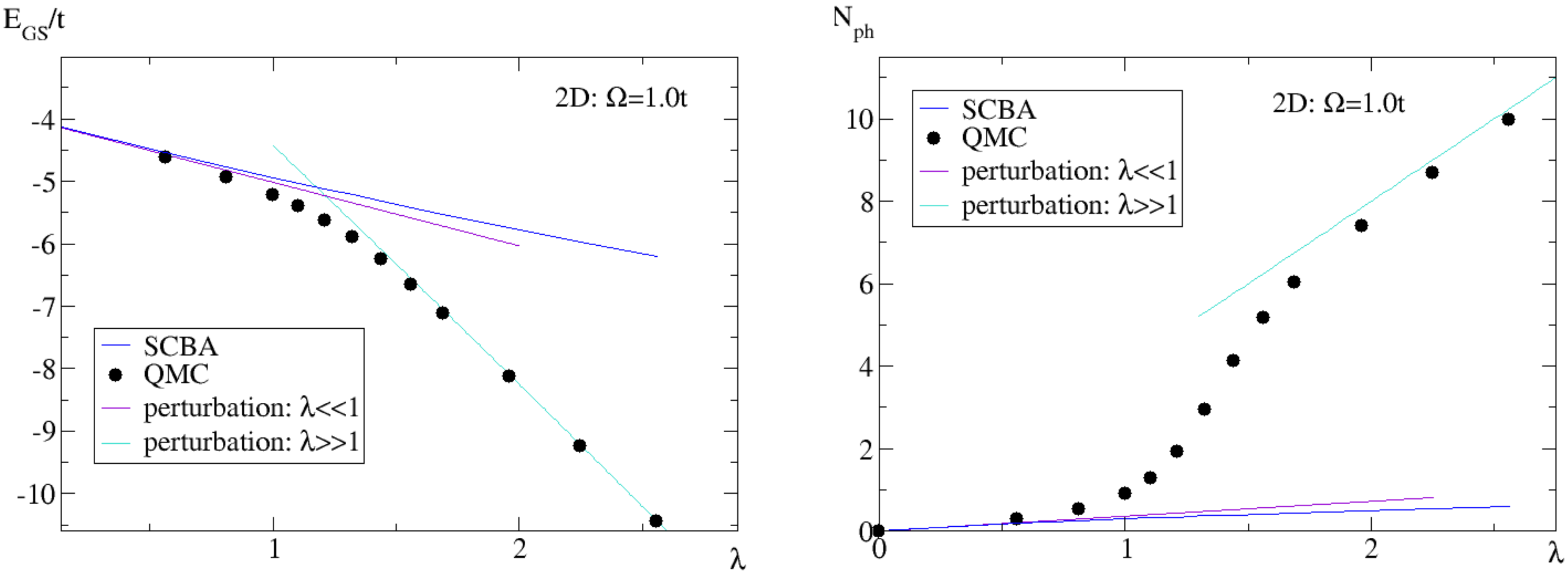


Single polaron in the 2D Holstein model

$$\lambda = \frac{g^2}{2dt\Omega}$$

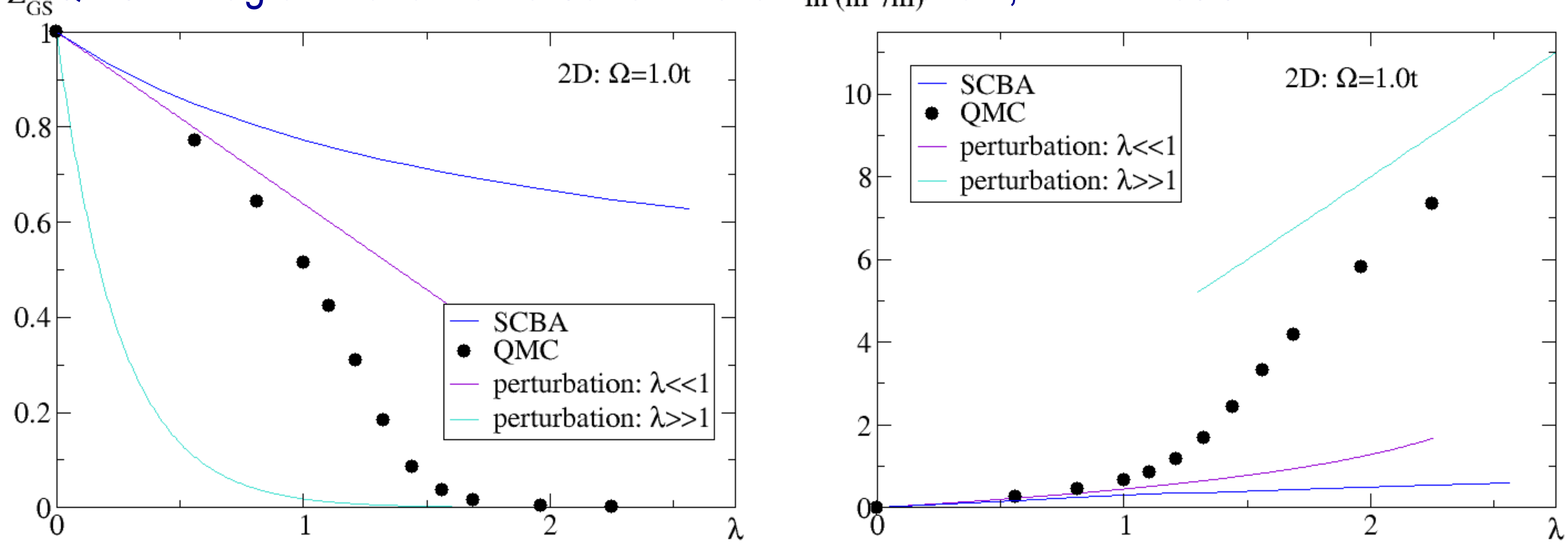


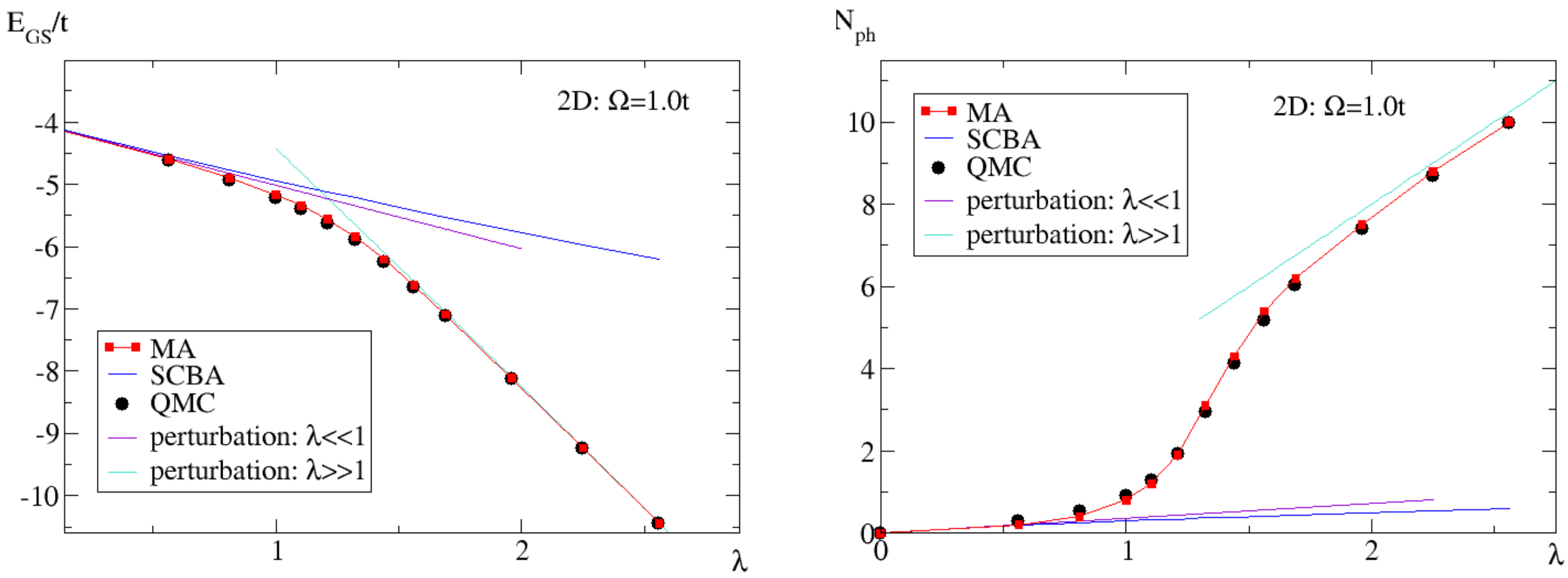




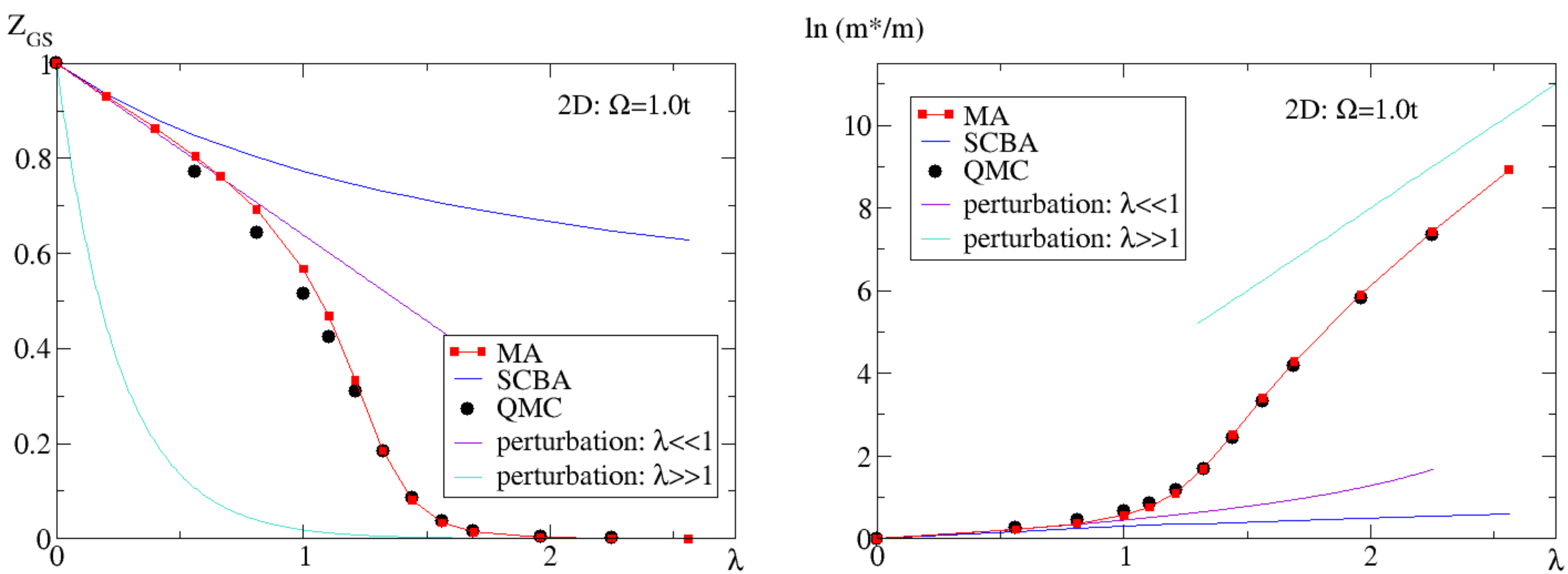
SCBA – leading analytic approx. at the time

QMC = Diagrammatic Monte Carlo : Alexandru Macridin, Ph.D. thesis





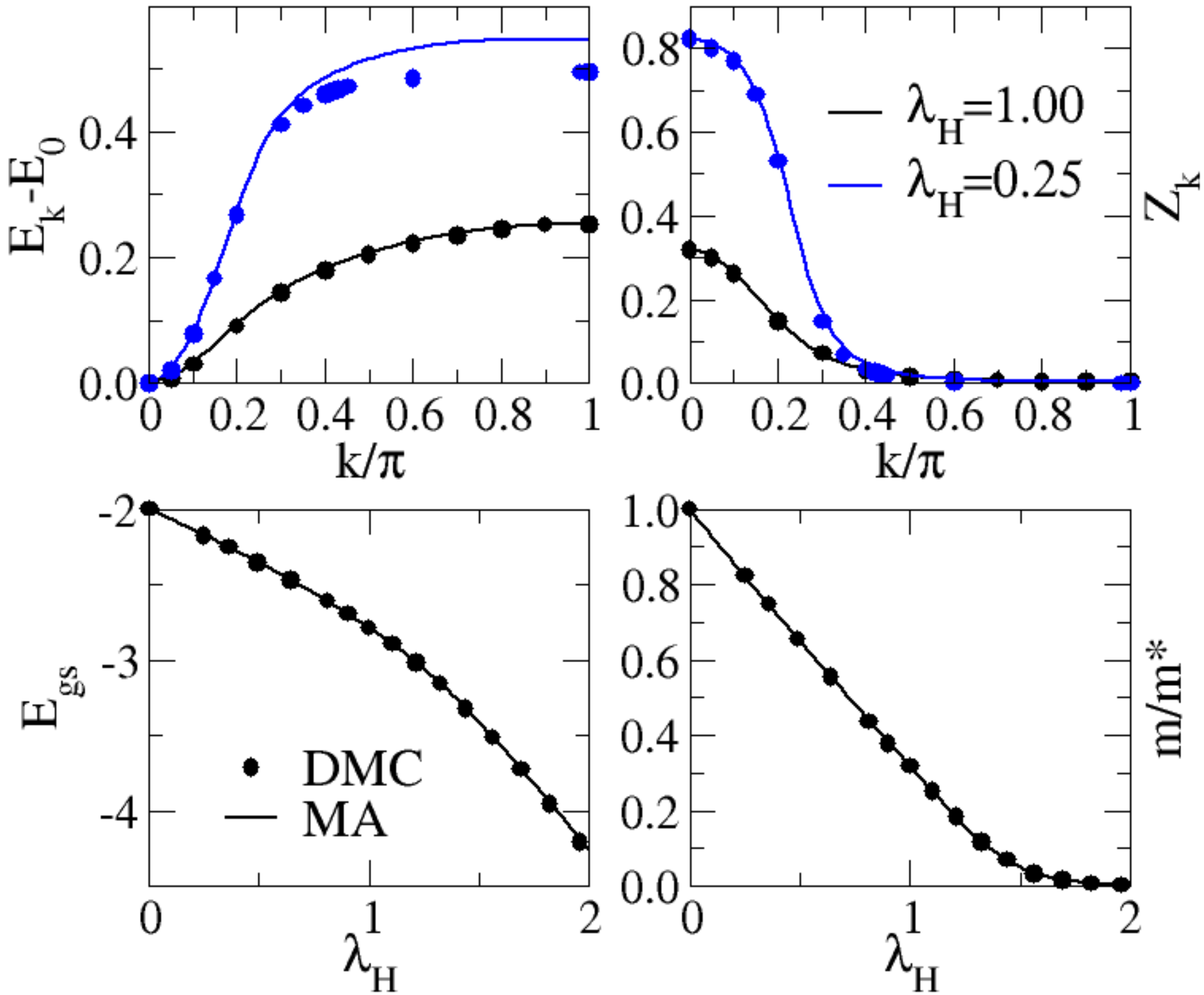
Momentum Average= MA = variational method, **M. Berciu, Phys.Rev.Lett. 97, 036402 (2006)**



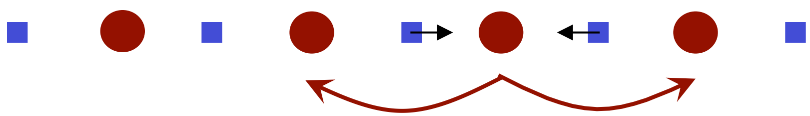
Single polaron in the 1D Holstein model

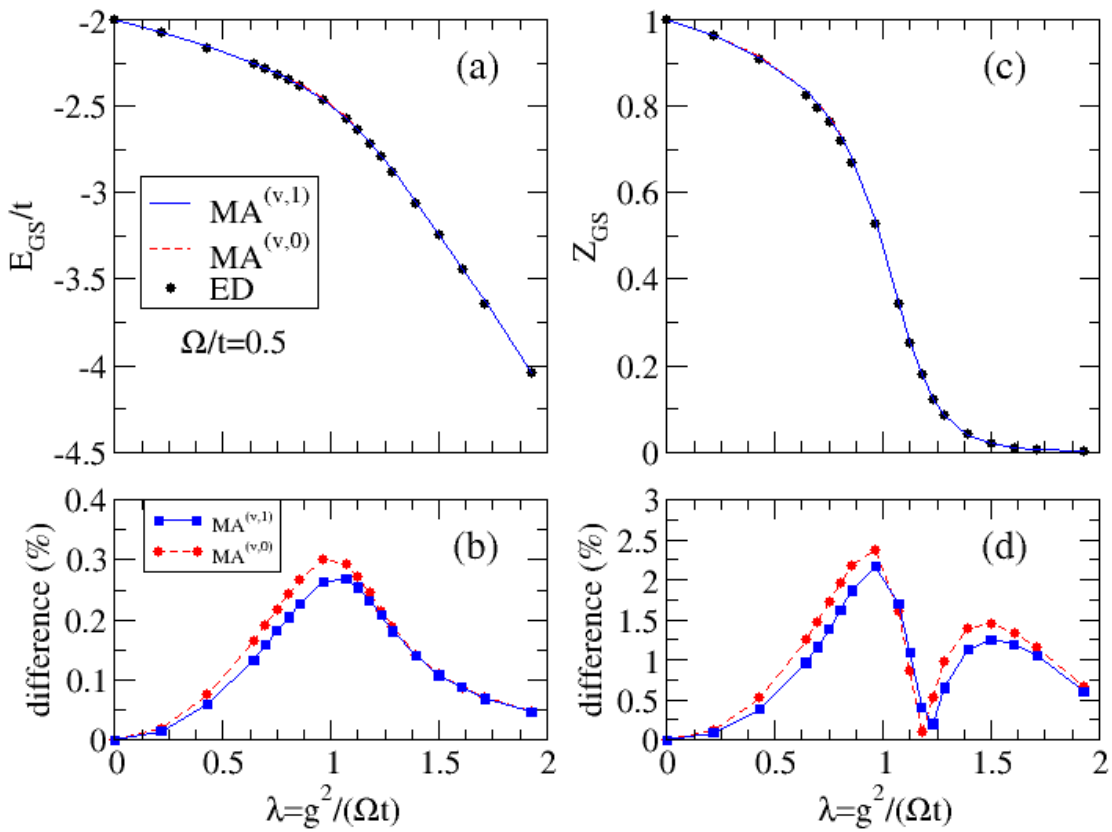
circles = DMC

lines = MA



Single polaron in 1D Breathing-Mode phonon coupling model:





MA: need a 2-site cloud **G. L. Goodvin and M. Berciu, PRB 78, 235120 (2008)**

Numerics: **Bayo Lau, M. Berciu and G. A. Sawatzky, Phys. Rev. B 76, 174305 (2007)**

Vey brief summary of the research from most of these past 80 years:

All models studied (Holstein, coupling to breathing-mode phonon, Frohlich, …) show qualitatively similar results →

The “polaron paradigm”: the stronger the coupling, the bigger the dressing cloud, the heavier the polaron.

Not surprising, because in all these models the phonons modulate the potential energy of the particle, therefore stronger coupling = a bigger cloud = deeper potential well = harder for the particle to “climb out” of it and move to the next site.

Rather boring: if el-ph coupling large enough to lead to something interesting (eg, strong pairing → high-T_c superconductivity), polaron mass is huge and any disorder or inhomogeneity will localize them.

But: phonons also modulate the kinetic energy of the particle!

Phonon-modulated hopping like in polyacetylene (Su-Schrieffer-Heeger or Peierls coupling)

$$t_{i,i+1} \propto e^{-(R_{i+1}-R_i)/a_B} = t e^{-(u_{i+1}-u_i)/a_B} \approx t - \alpha(u_{i+1}-u_i)$$

Single polaron in the 1D SSH model

Circles – MA;

Lines – BDMC, D. Marchand and P. Stamp

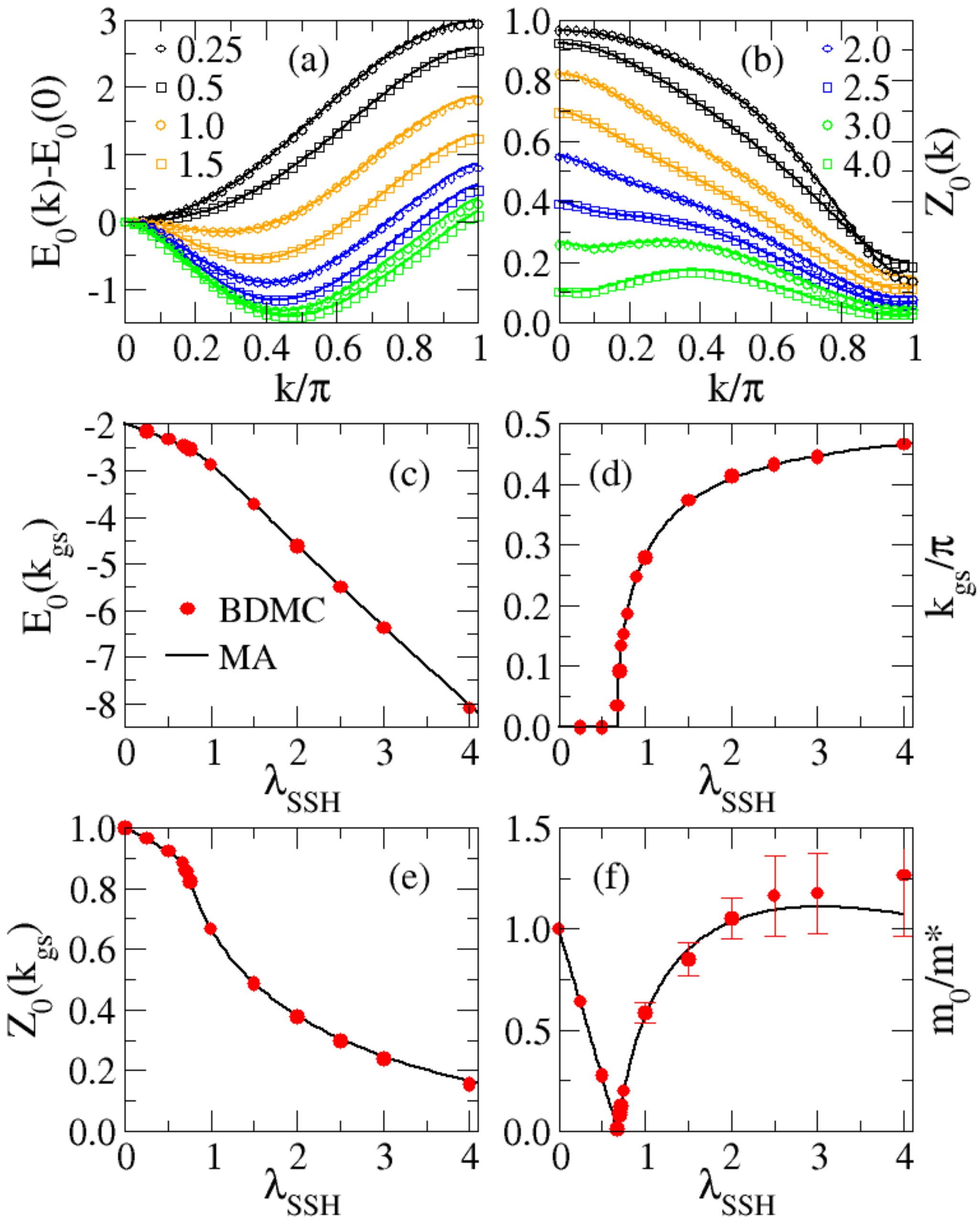
Also very good agreement with data from G. de Filippis + V. Cataudella and A. Mishchenko + N. Nagaosa, **PRL 105, 266605 (2010)**

Momentum of GS switches from 0 (weak coupling, non-degenerate GS) to finite value (strong coupling, doubly-degenerate GS)

→ True transition (not crossover) from large to small polaron

→ Such transitions are impossible in if the potential energy is modulated

→ above the transition, the polaron is light even for strong coupling and has an unusual dispersion



New polaronic behavior (also verified in Edwards in t-J_z models):

Unlike for models where the bosons modulate the potential energy (→ stronger coupling → bigger distortion = deeper potential well → harder to move), in models where the bosons modulate the kinetic energy:

-- polarons can be very light even at very strong coupling because hopping integrals can be larger in the presence of phonons

-- sharp transitions are possible in such models (they are impossible in the other class of models **B. Gerlach and H. Lowen, Rev. Mod. Phys. 63, 63 (1991)**)

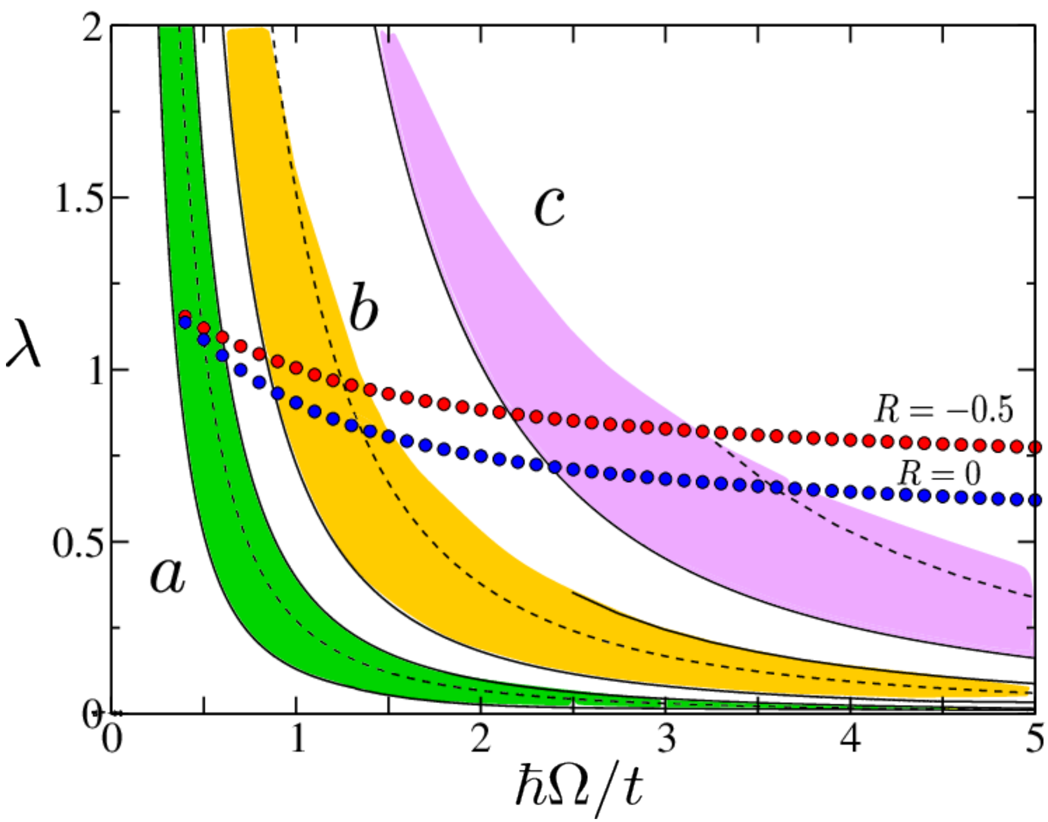
-- polaron dispersion can be quite different from that of the bare particle → may be possible to engineer various macroscopic properties

How about in mixed models (both types of coupling)?

Holstein + SSH (**with Dominic and Philip**)

BM + SSH (**F. Herrera, K. Madison, R. Krems and M. Berciu, PRL 110, 223003 (2013)**)

Proposal: polar molecules trapped one-per-site in an optical lattice. The "particle" is an exciton (molecule excited from l=0 gs to l=1 excited state) whose on-site and kinetic energies are modulated by dipole-dipole interactions. Phonons are the vibrations of each molecule in its trap.



a: LiCs (large dipole moment)

b: RbCs (medium dipole moment)

c: KRb (small dipole moment)

R= ratio of BM/SSH coupling

MA – happy to discuss technical details with anybody interested

→ generate BBGKY hierarchy of equations of motion for the propagator using a variational principle. Here: over how many adjacent sites is the cloud allowed to extend. Holstein = 1, BM = 2, Edwards model = 3, etc …

→ can improve systematically by enlarging the space (but more work)

→ has been generalized with equal success to systems with disorder and inhomogeneity (**M. Berciu, A. Mischchenko and N. Nagaosa, EPL 89, 37007 (2010); H. Ebrahimnejad and M. Berciu, PRB 85, 165117 (2012) and PRB 86, 205109 (2012); G. L. Goodvin, L. Covaci and M. Berciu, PRL 107, 076403 (2011)**)

→ has also been generalized to "biased" systems, where phonons must be emitted in order for the particle to be able to move to lower energies (**A. Cheung and M. Berciu, PRB 88, 035132 (2013)**)

→ has also been generalized to calculating response functions, eg. optical absorption **(G. L. Goodvin, A. S. Mischchenko, M. Berciu, PRL 107, 0763403 (2011))**

→ has also been generalized to non-linear coupling models (**C. Adolphs and M. Berciu, EPL 102, 47003 (2013) and PRB 89, 035122 (2014)**)

Conclusions:

→ In solid-state systems, the effects of coupling to bosons depend qualitatively on what type of coupling dominates (modulating potential vs. kinetic energy)

→ Extremely likely that similar considerations apply to modeling biological systems