The Green's function of a Holstein polaron

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Numerical data: A. Macridin, Bayo Lau, V. Cataudella, P. Kornilovitch

More details: M. Berciu, Phys. Rev. Lett. 97, 036402 (2006)
G. Goodvin, M. Berciu and G. Sawatzky, Phys. Rev. B 74, 245104 (2006)
M. Berciu, Phys. Rev. Lett. 98, 209702 (2007)
M. Berciu and G. Goodvin, Phys. Rev. B 96, 165109 (2007)

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(Very general) motivation:

Generically, $H = \alpha\, H_1 + \beta\, H_2$

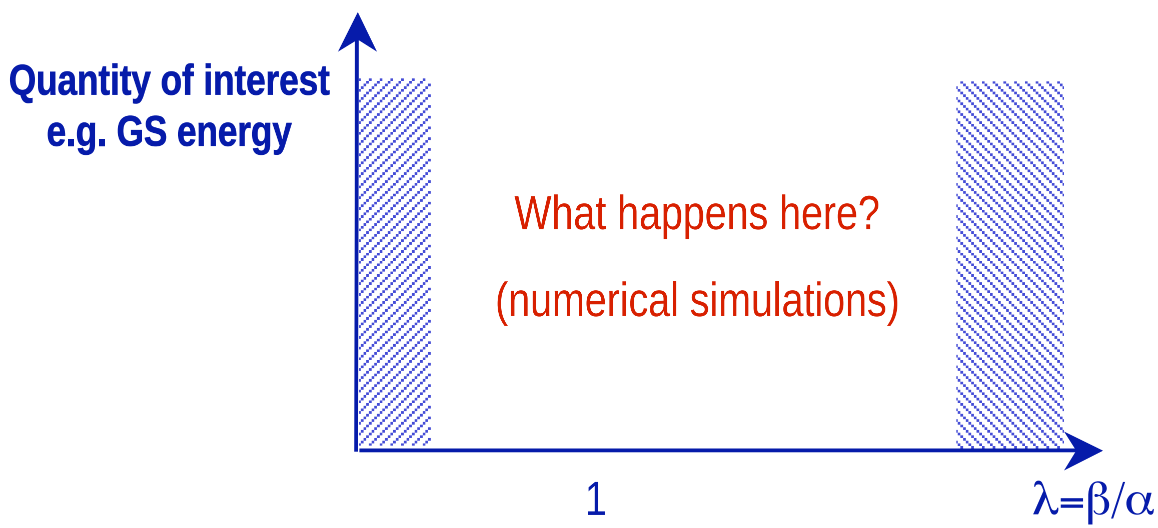
characteristic energy scale

Very often, ground-state of H_1 is VERY different from ground-state of H_2.

How about ground-state of H, what does it look like ? (from now on, GS = ground-state)

If $\beta \ll \alpha$, $H = \alpha\,(H_1 + \lambda\, H_2)$, with $\lambda=\beta/\alpha \ll 1$ → do perturbation in λ

If $\alpha \ll \beta$, $H = \beta\,(H_2 + \lambda^{-1}\, H_1)$, with $\lambda^{-1}=\alpha/\beta \ll 1$ → do perturbation in $1/\lambda$



In this talk: for a particular problem (Holstein polaron) → one analytical approx. that works well for all λ.

Hopefully it will prove possible to generalize this to other systems.

Polarons: (first) model of interest: the Holstein Hamiltonian

The simplest lattice Hamiltonian describing electron-phonon (phonons = lattice vibrations) interactions:

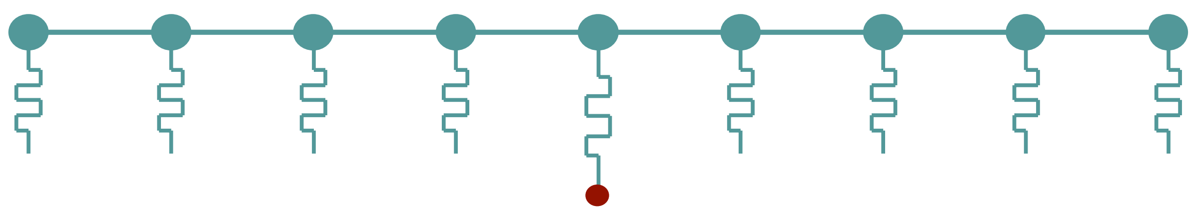
$$H = -t \sum_{<i,j>} (c_{i\sigma}^{+} c_{j\sigma} + c_{j\sigma}^{+} c_{i\sigma}) + \Omega \sum_i b_i^{+} b_i + g \sum_i n_i (b_i^{+} + b_i)$$

$$b_i^{+} + b_i \propto \hat{x}_i - x_0$$

→ 2 dimensionless parameters:

$$\lambda = \frac{g^2}{2dt\Omega}; \quad \frac{\Omega}{4dt}$$

Suppose we have a single electron in the system:



Eigenstates are linear combinations of states with electron at different sites, surrounded by a lattice distortion (cloud of phonons) in its vicinity.

This composite object: electron dressed by surrounding cloud of phonons is called a polaron. We would like to learn its properties: for e.g., the stronger the el-ph interactions are (larger λ), the bigger this cloud/deformation is → the slower (heavier) the polaron.

(Landau, 1933. Holstein model proposed in 1959).

Quantity of interest: the Green's function G(k,ω) and the spectral weight A(k,ω)

Main idea: if you want to learn something about what's going on in an unknown place, send in spies!
Here: add one extra particle (electron) in the system of interest, and extract it at a later time

$G(r_2,t_2;r_1,t_1) = \textit{amplitude of probability}$ that an electron introduced in the system at r_1, t_1 will be found at a later time $t_2 > t_1$ time at r_2.

If the system is invariant to translations, it is more convenient to work with energy and momentum, then with time and spatial location → work with Fourier transform G(k,ω)

$$H\left|1,k,\alpha\right\rangle = E_{1,k,\alpha}\left|1,k,\alpha\right\rangle$$

← eigenenergies and eigenfunctions (1 electron, total momentum k, α is collection of other quantum numbers)

$$G(k,\omega) \square \left\langle 0\right| c_k \frac{1}{\omega - H + i\eta} c_k^+ \left|0\right\rangle = \sum_\alpha \frac{Z_{1,k,\alpha}}{\omega - E_{1,k,\alpha} + i\eta}$$

$$Z_{1,k,\alpha} = \left|\left\langle 1,k,\alpha\right| c_k^+ \left|0\right\rangle\right|^2$$

$$A(k,\omega) \square -\frac{1}{\pi}\,\mathrm{Im}\,G(k,\omega)$$

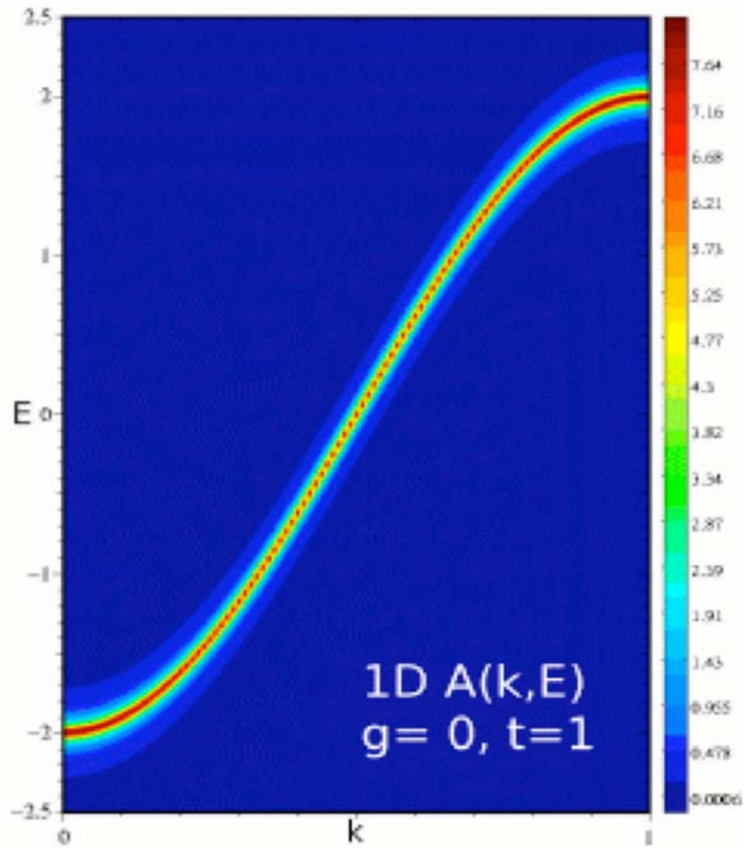
← is measured by (inverse) angle-resolved photoemission spectroscopy = ARPES weak coupling $\lambda = \frac{g^2}{2dt\Omega} = 0 \quad (g = 0)$

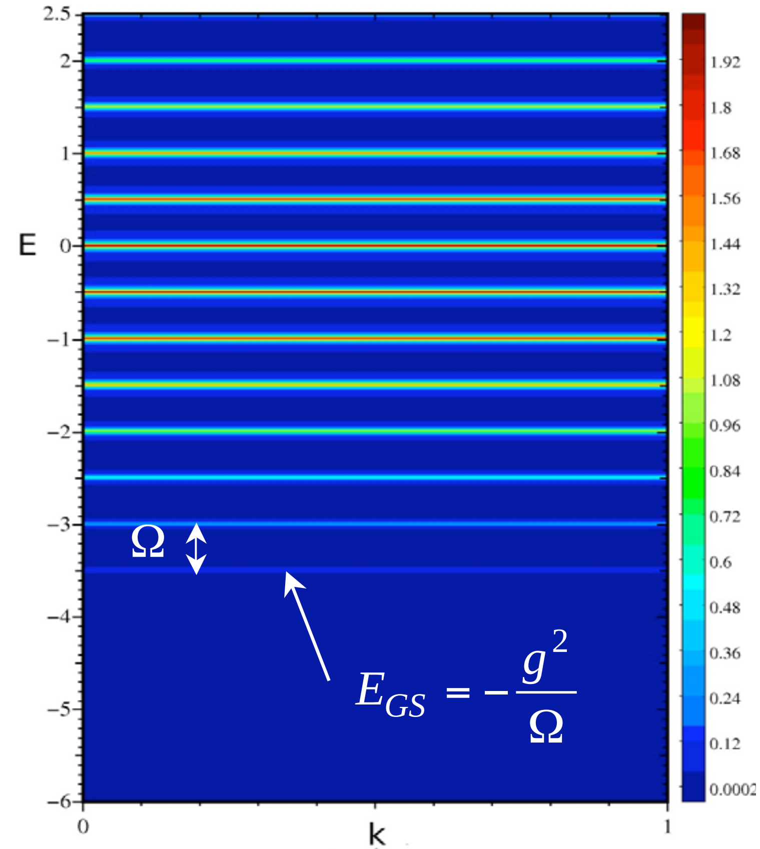
$$G_0(k,\omega) = \frac{1}{\omega - \varepsilon_k + i\eta};$$

$$A_0(k,\omega) = \frac{\eta}{\pi\left[\left(\omega - \varepsilon_k\right)^2 + \eta^2\right]} \xrightarrow{\eta \to 0} \delta\left(\omega - \varepsilon_k\right)$$

Lang-Firsov impurity limit $\lambda = \frac{g^2}{2dt\Omega} = \infty \quad (t = 0)$

$$G_{LF}(k,\omega) = e^{-\frac{g^2}{\Omega^2}} \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{g}{\Omega}\right)^{2n} \frac{1}{\omega + \frac{g^2}{\Omega} - n\Omega + i\eta}$$





How does the spectral weight evolve between these two very different limits?

Calculating the Green's function:

$$G(k,\omega) = \frac{1}{\omega - \varepsilon_k - \Sigma(k,\omega) + i\eta} \qquad G_0(k,\omega) = \frac{1}{\omega - \varepsilon_k + i\eta}$$

$\Sigma(k,\omega) =$  +....

For Holstein polaron, we need to sum to orders well above g^2/Ω^2 to get convergence.

n	1	2	3	4	5	6	7	8
Σ, exact	1	2	10	74	706	8162	110410	1708394
Σ, SCBA	1	1	2	5	14	42	132	429

Traditional approach: find a subclass of diagrams that can be summed, ignore the rest

→ self-consistent Born approximation (SCBA) – sums only non-crossed diagrams (much fewer)

New proposal: the MA$^{(n)}$ hierarchy of approximations:

Idea: keep ALL self-energy diagrams, but approximate each such that the summation can be carried out analytically. (Alternative explanation: generate the infinite hierarchy of coupled equations of motion for the propagator, keep all of them instead of factorizing and truncating, but simplify coefficients so that an analytical solution can be found).

First: MA$^{(0)}$ – simplest (least accurate) version

Replace each in the self-energy diagrams by

$G_0(\vec{k},\omega)$

$$g_0(\omega) = \frac{1}{N}\sum_k G_0(\vec{k},\omega)$$

→ one can sum all the resulting self-energy diagrams:

$$= \int_{B.Z.} \frac{d\vec{k}}{(2\pi)^d}\frac{1}{\omega - \varepsilon_{\vec{k}} + i\eta}$$

Define continued fractions: $A_n(\omega) = \dfrac{n g_0(\omega - n\Omega)}{1 - g^2 g_0(\omega - n\Omega) A_{n+1}(\omega)}, \quad A_{n\to\infty} \to 0$

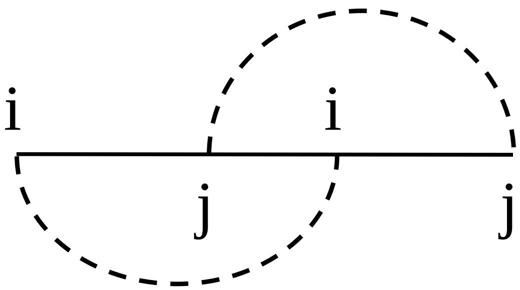
$$\Sigma_{MA^{(0)}}(\omega) = g^2 A_1(\omega) = \cfrac{g^2 g_0(\omega-\Omega)}{1 - \cfrac{2g^2 g_0(\omega-\Omega) g_0(\omega-2\Omega)}{1 - \cfrac{3g^2 g_0(\omega-2\Omega) g_0(\omega-3\Omega)}{\ldots}}}$$

← result is EXACT both for g=0 and for t=0

← trivial to evaluate

Why should this be a reasonable thing to do?

(i) Real-space argument: $MA^{(0)}$ means $G_0(i-j,\omega-n\Omega) \rightarrow \delta_{i,j} G_0(0,\omega-n\Omega) = \delta_{i,j} g_0(\omega-n\Omega)$



$$exact: \quad g^4 \sum_{i,j} G_0(j-i,\omega-\Omega) G_0(i-j,\omega-2\Omega) G_0(j-i,\omega-\Omega)$$

$$MA^{(0)}: \quad g^4 g_0(\omega-\Omega) g_0(\omega-2\Omega) g_0(\omega-\Omega)$$

At low energies $\omega \sim E_{GS} < -2dt$ → free electron Greens' functions decrease *exponentially* with distance $|i-j|$ → $MA^{(0)}$ keeps the most important (diagonal) contribution. The approximation becomes better the more phonons are present, since the lower $\omega - n\,\Omega$ is, the faster the decay.

→ Expect ground-state properties to be described quite accurately.

(ii) Spectral weight sum rules (see PRB 74, 245104 (2006) for details)

$$M_n(k) = \int_{-\infty}^{\infty} d\omega\, \omega^n A(k,\omega) = -\frac{1}{\pi} \mathrm{Im} \int_{-\infty}^{\infty} d\omega\, \omega^n G(k,\omega)$$

← can be calculated exactly

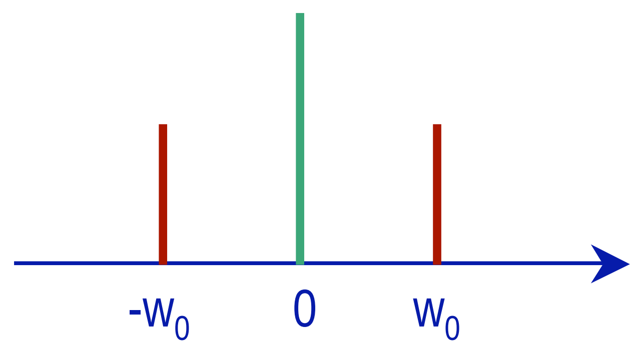
$$M_n(k) = \langle 0 | c_k H^n c_k^+ | 0 \rangle$$

MA$^{(0)}$ satisfies exactly the first 6 sum rules, and with good accuracy all the higher ones.

Note: it is not enough to only satisfy a few sum rules, even if exactly. ALL must be satisfied as well as possible.

Examples: 1. SCBA satisfies exactly the first 4 sum rules, but is very wrong for higher order sum rules → fails miserably to predict strong coupling behavior (proof coming up in a minute).

2. Compare these two spectral weights:



$$A_1(\omega) = \delta(\omega) \to M_0 = 1; M_{n>0} = 0$$

$$A_2(\omega) = \frac{1}{2}\big(\delta(\omega-\omega_0) + \delta(\omega+\omega_0)\big) \to M_n = \frac{\omega_0^n}{2}\left[1+(-1)^n\right] = 0, \quad \text{if n is odd}$$

$$M_n(k) = \int_{-\infty}^{\infty} d\omega \omega^n A(k,\omega) = -\frac{1}{\pi} \mathrm{Im} \int_{-\infty}^{\infty} d\omega \omega^n G(k,\omega)$$

Since G(k,w) is a sum of diagrams, keeping the correct no. of diagrams is extremely important!

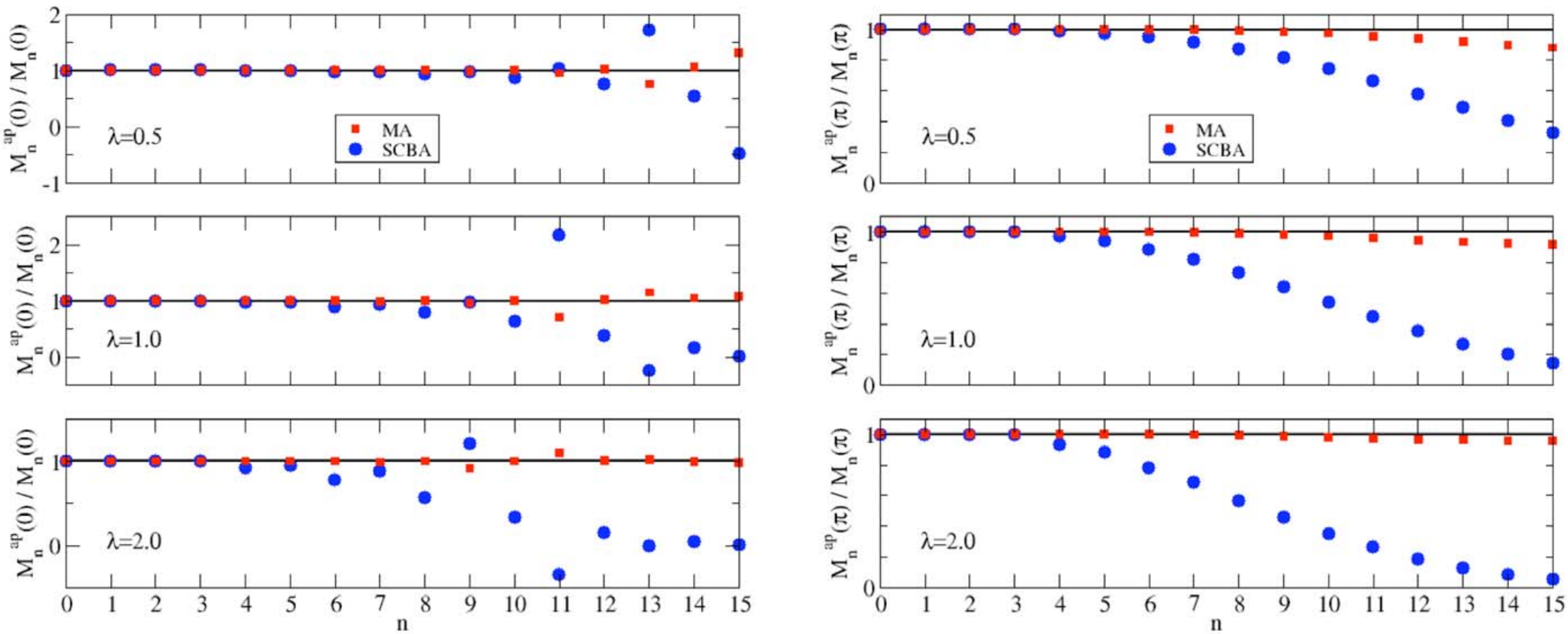
found correctly if n=0 diagram kept correctly → dominates if t >> g, λ → 0

$$M_6(\vec{k}) = \varepsilon_{\vec{k}}^6 + g^2[5\varepsilon_{\vec{k}}^4 + 6t^4\left(2d^2 - d\right) + 4\varepsilon_{\vec{k}}^3\Omega + 3\varepsilon_{\vec{k}}^2\Omega^2 + 6dt^2(\varepsilon_{\vec{k}}^2 + \varepsilon_{\vec{k}}\Omega + 2\Omega^2)$$
$$+ 2\varepsilon_{\vec{k}}\Omega^3 + \Omega^4] + g^4\left[18dt^2 + 12\varepsilon_{\vec{k}}^2 + 22\varepsilon_{\vec{k}}\Omega + 25\Omega^2\right] + 15g^6$$

found correctly if we sum correct no. of diagrams → dominates if g >>t, λ >>1

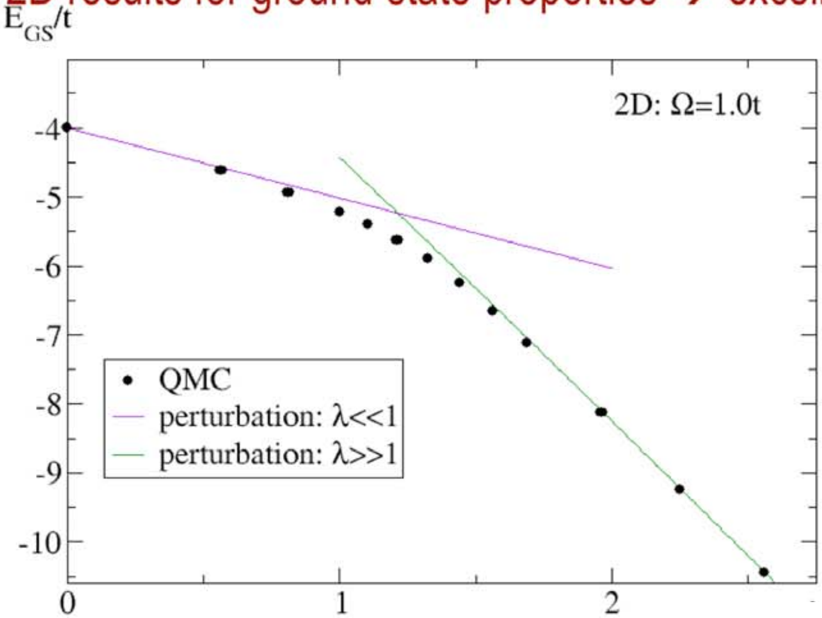
$$M_{6,MA}(\vec{k}) = M_6(\vec{k}) - 2dt^2g^4$$

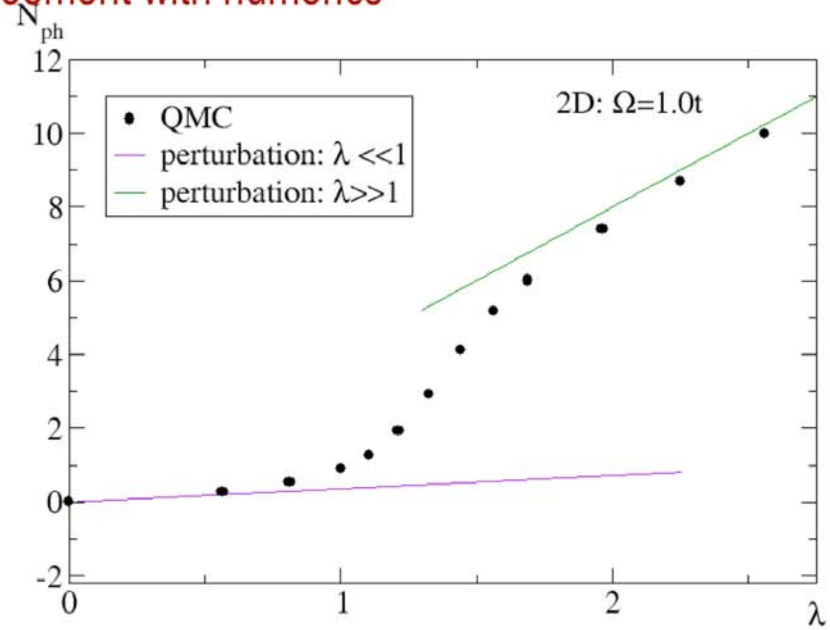
$$M_{6,SCBA}(\vec{k}) = M_6(\vec{k}) - g^4\left[....\right] - 10g^6$$



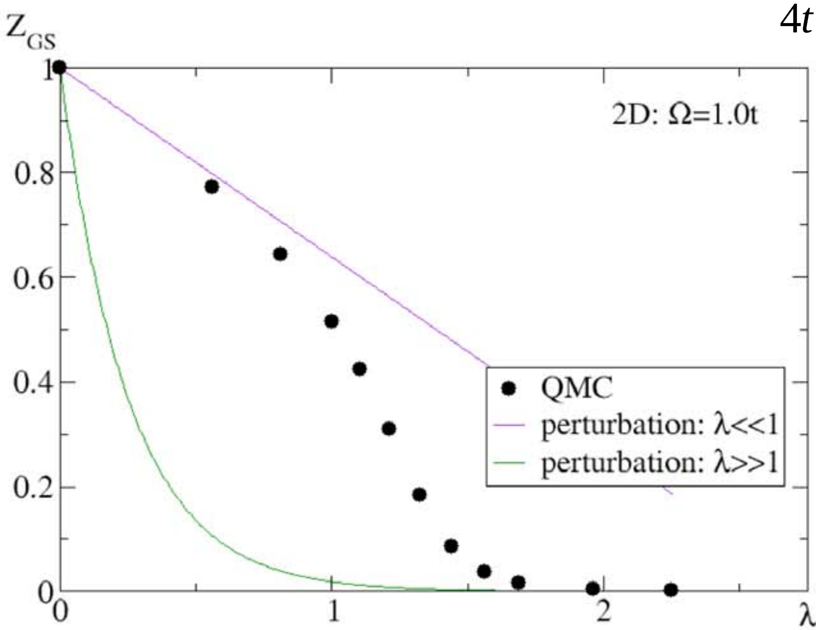
$$\lambda = \frac{g^2}{2dt\Omega}$$

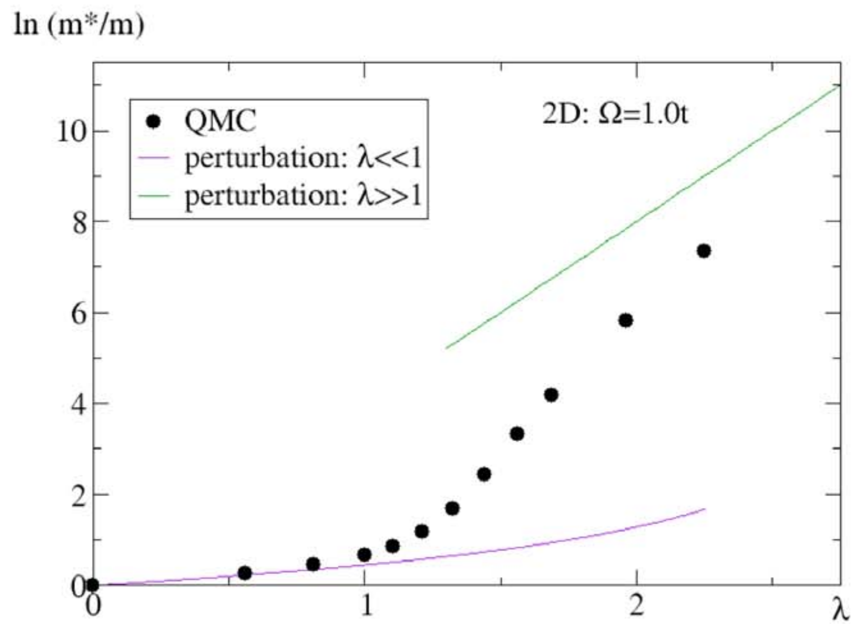
2D results for ground-state properties → excellent agreement with numerics

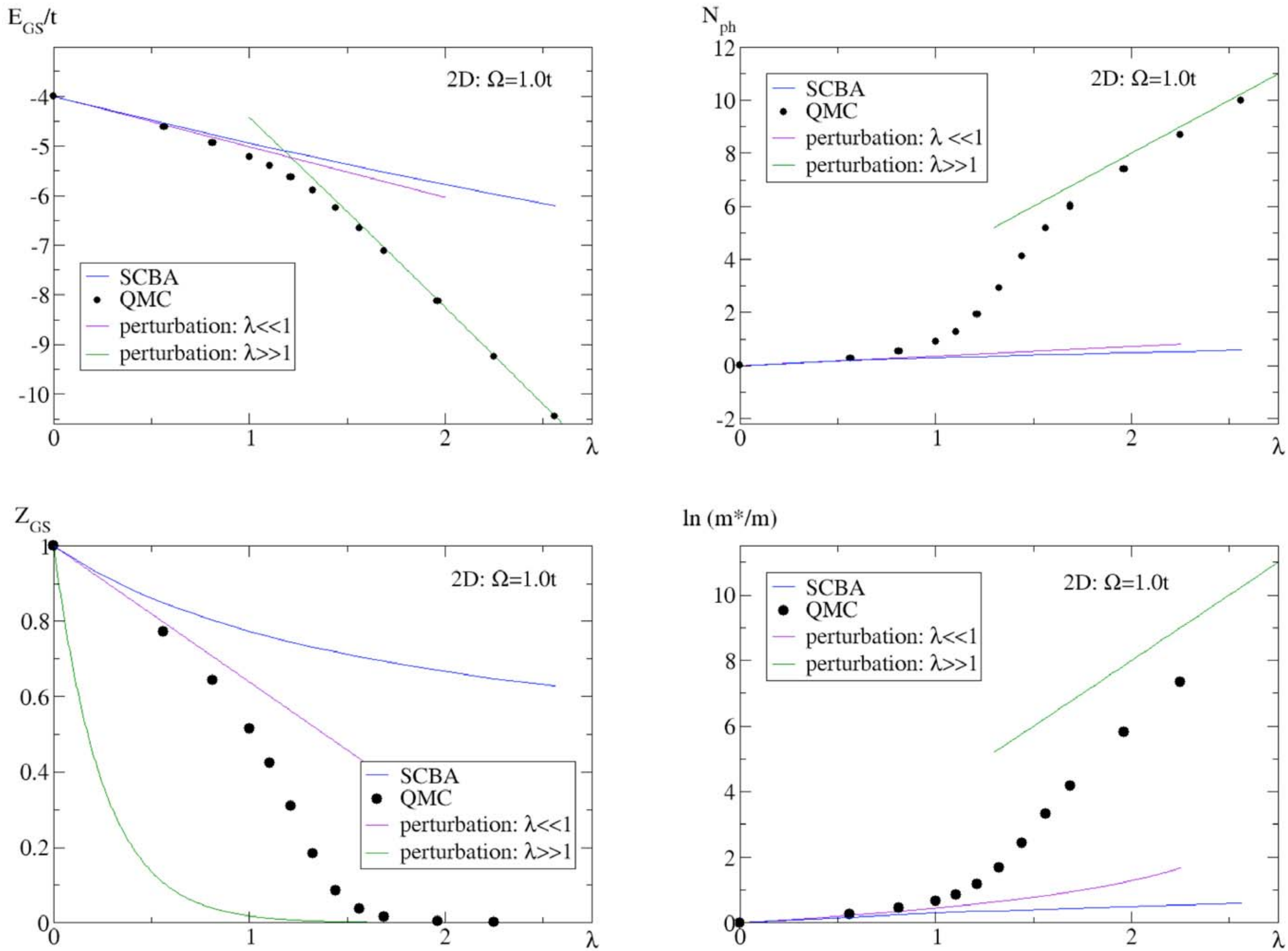




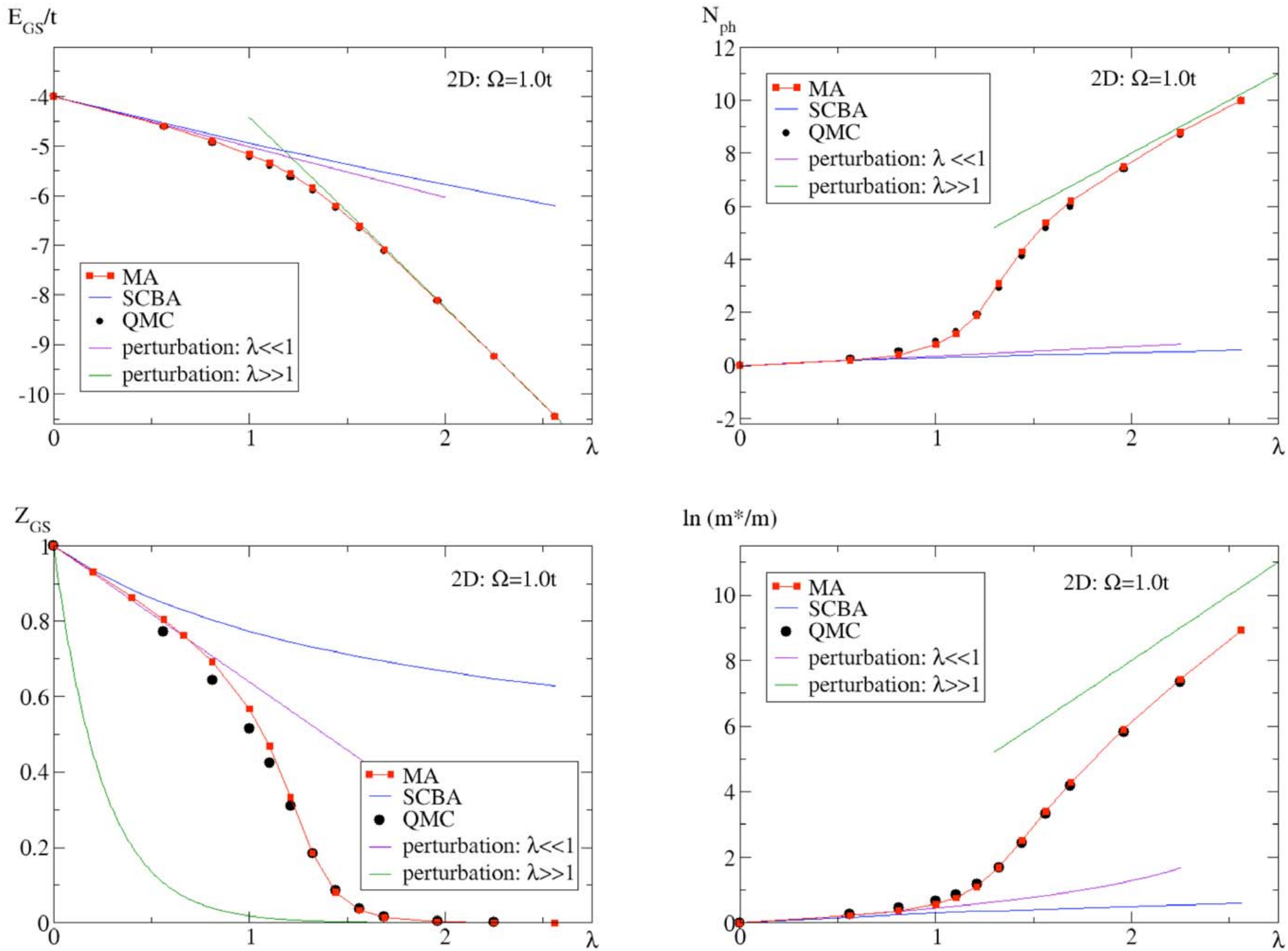
$$\lambda = \frac{g^2}{4t\Omega}$$





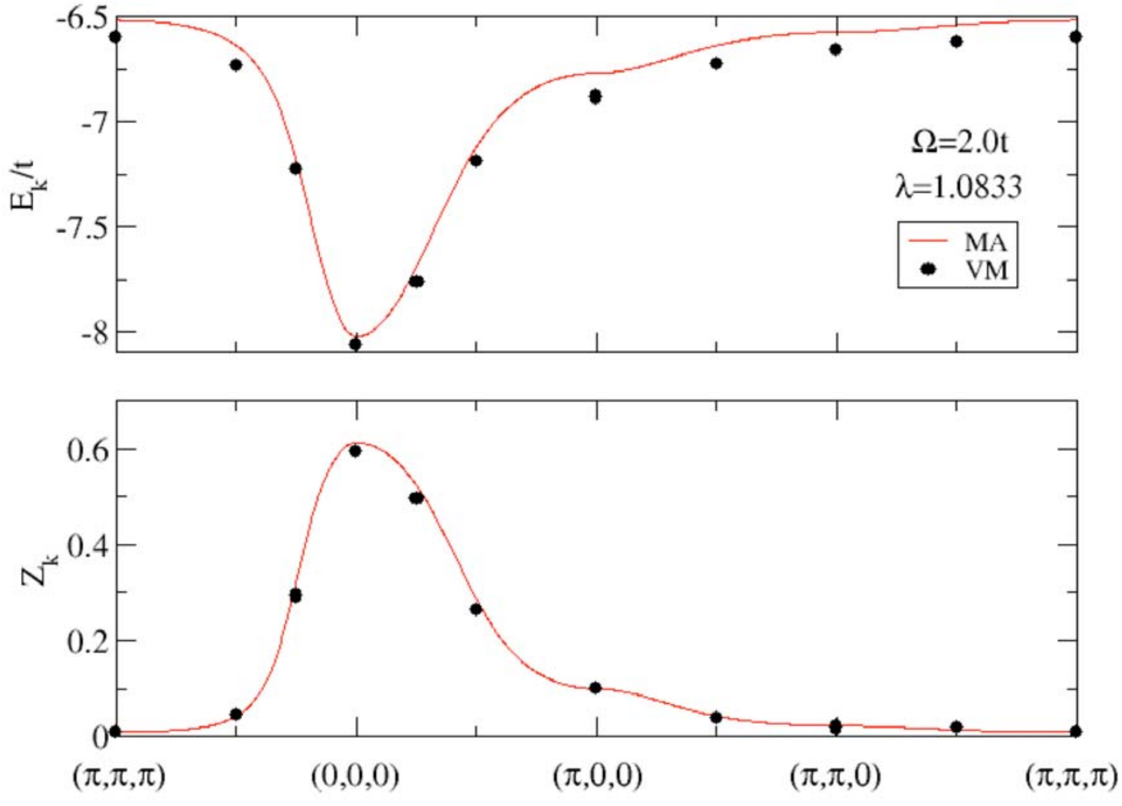


E_GS/t
2D: Ω=1.0t
SCBA
QMC
perturbation: λ<<1
perturbation: λ>>1
-4
-5
-6
-7
-8
-9
-10
0
1
2
λ
N_ph
2D: Ω=1.0t
SCBA
QMC
perturbation: λ <<1
perturbation: λ>>1
12
10
8
6
4
2
0
-2
0
1
2
λ
Z_GS
2D: Ω=1.0t
SCBA
QMC
perturbation: λ<<1
perturbation: λ>>1
1
0.8
0.6
0.4
0.2
0
0
1
2
λ
ln (m*/m)
2D: Ω=1.0t
SCBA
QMC
perturbation: λ<<1
perturbation: λ>>1
10
8
6
4
2
0
0
1
2
λ

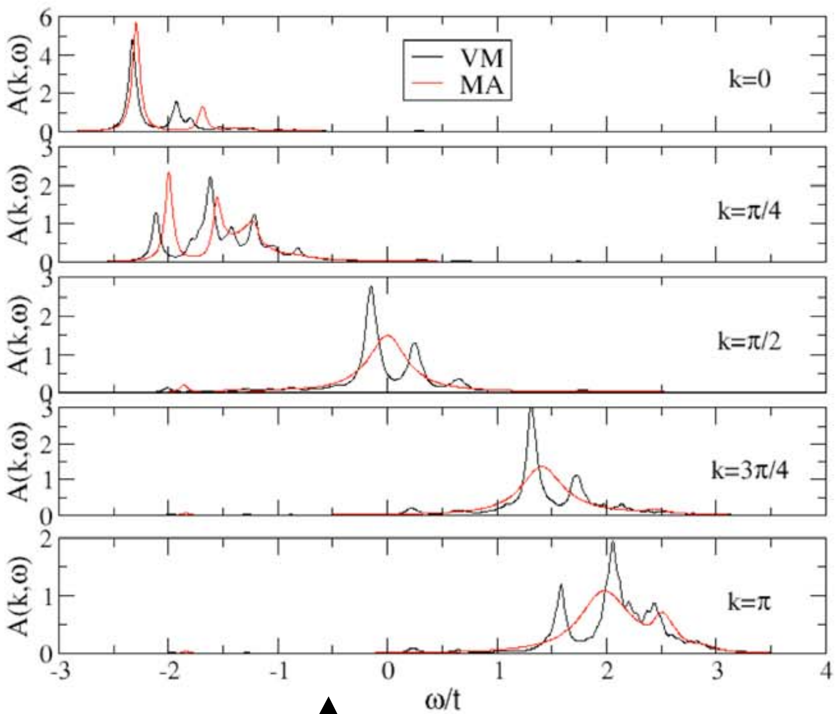


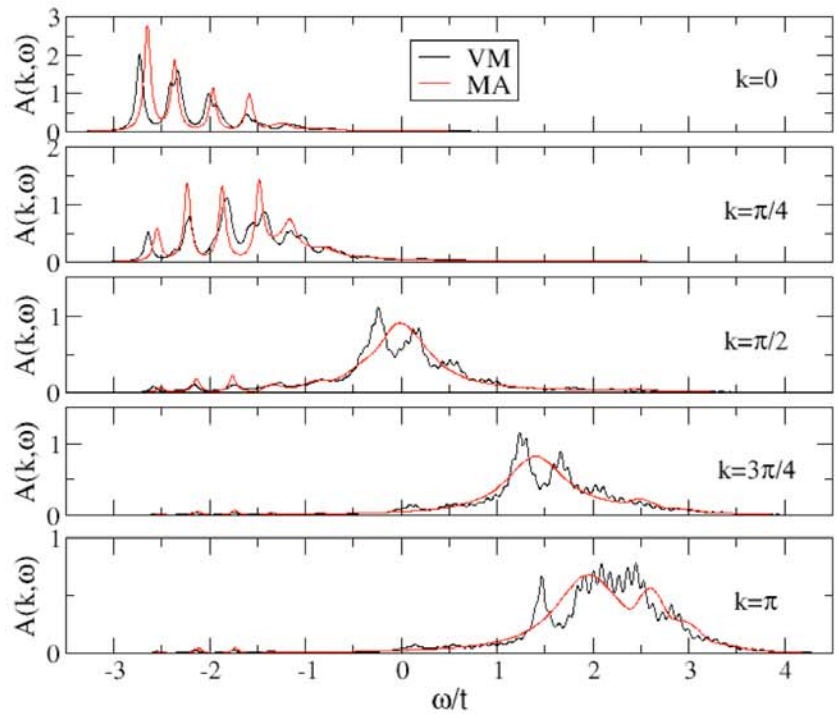
E_{GS}/t
2D: Ω=1.0t
MA
SCBA
QMC
perturbation: λ<<1
perturbation: λ>>1
-4
-5
-6
-7
-8
-9
-10
0
1
2
λ
N_{ph}
12
10
8
6
4
2
0
-2
Z_{GS}
1
0.8
0.6
0.4
0.2
ln (m*/m)

3D Polaron dispersion



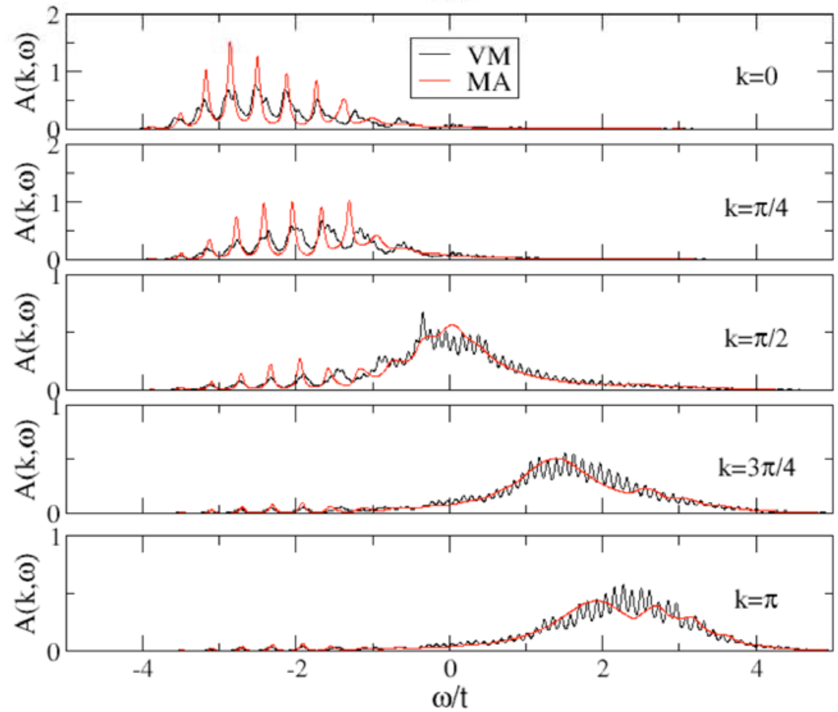
L. -C. Ku, S. A. Trugman and S. Bonca, Phys. Rev. B 65, 174306 (2002).





λ = 0.5

λ = 1



λ = 2

A(k,ω) in 1D

G. De Filippis et al, PRB 72, 014307 (2005)

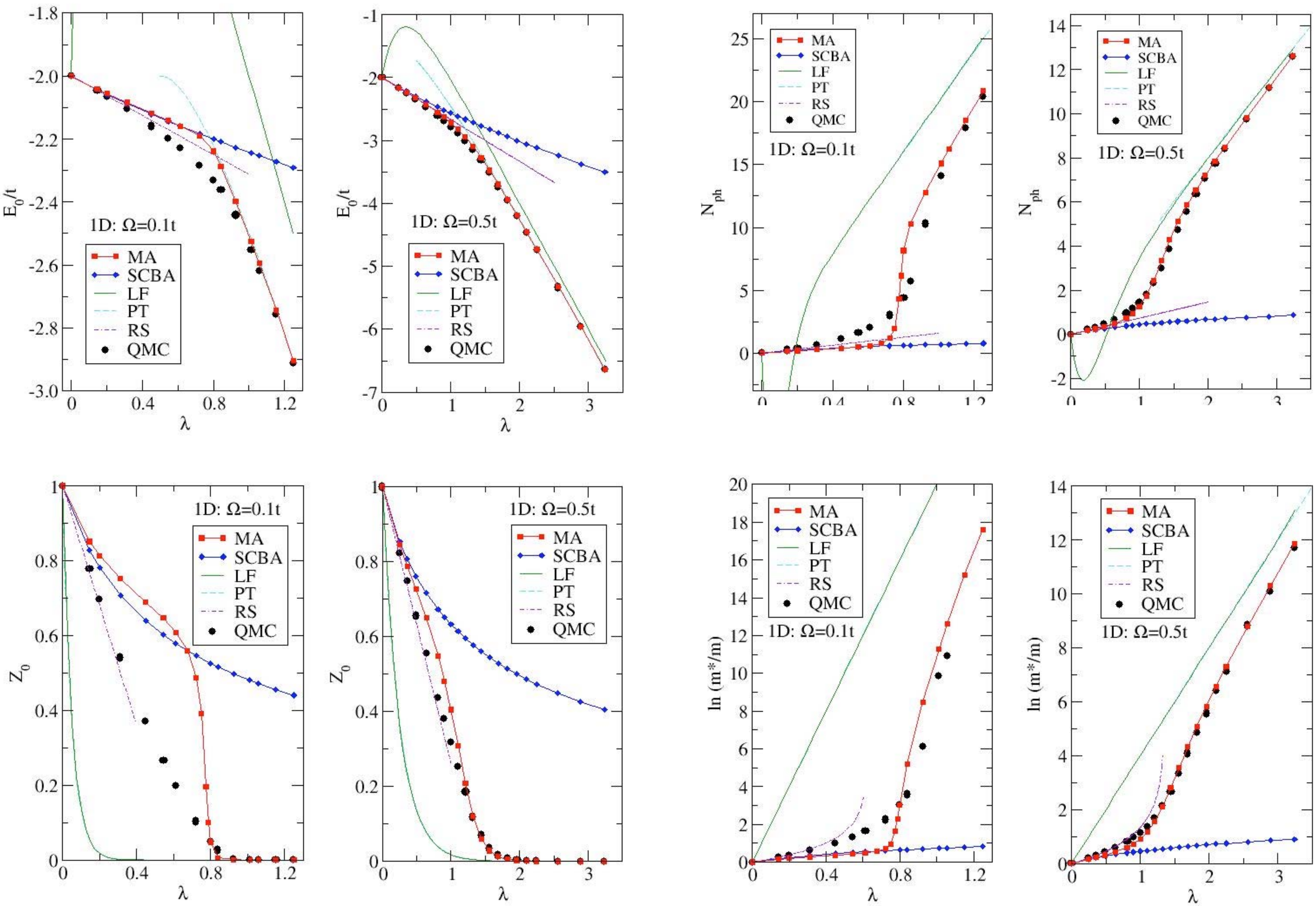
MA becomes exact for small, large λ

For lots more comparisons against available numerics, see PRB 74, 245104 (2006).

Conclusion so far: $MA^{(0)}$ is remarkably good, especially considering how simple it is. However, it is an approximation, and it does have its problems:

→ self-energy is momentum independent!

→ the accuracy worsens if $\Omega/t \rightarrow 0$



E0/t
λ
1D: Ω=0.1t
MA
SCBA
LF
PT
RS
QMC
E0/t
λ
1D: Ω=0.5t
MA
SCBA
LF
PT
RS
QMC
Nph
MA
SCBA
LF
PT
RS
QMC
1D: Ω=0.1t
Nph
MA
SCBA
LF
PT
RS
QMC
1D: Ω=0.5t
Z0
λ
1D: Ω=0.1t
MA
SCBA
LF
PT
RS
QMC
Z0
λ
1D: Ω=0.5t
MA
SCBA
LF
PT
RS
QMC
ln (m*/m)
λ
MA
SCBA
LF
PT
RS
QMC
1D: Ω=0.1t
ln (m*/m)
λ
MA
SCBA
LF
PT
RS
QMC
1D: Ω=0.5t

For lots more comparisons against available numerics, see PRB 74, 245104 (2006).

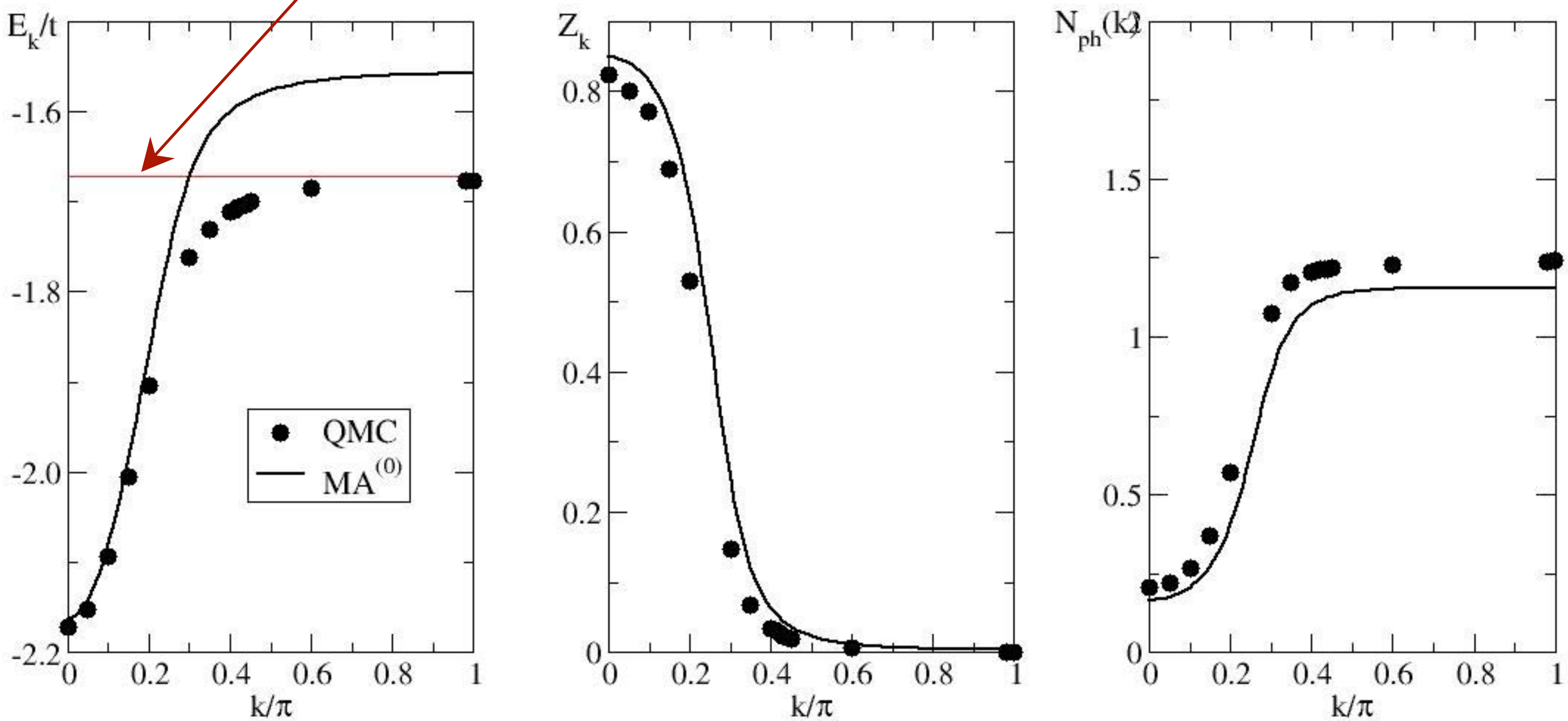
Conclusion so far: MA$^{(0)}$ is remarkably good, especially considering how simple it is. However, it is an approximation, and it does have its problems:

→ self-energy is momentum independent!

→ the accuracy worsens if $\Omega/t \to 0$

→ wrong location (at weak coupling) or outright absence (moderate and strong coupling) of the polaron+one-phonon continuum: this must always appear at precisely $E_{GS}+\Omega$.

$E_{GS} + \Omega$ – continuum starts above this energy



1D, Ω =0.5t, λ =0.25

Improve the approximation:

$MA^{(n)}$ keep free propagators of frequency $\omega - m\Omega$, $m < n$ exactly in the self-energy diagrams; all propagators with more phonons (lower energy) are momentum averaged

$MA^{(1)}$ – $G_0(k\text{-}q,\omega-\Omega)$ contributions exact, lines with 2 or more phonons are momentum averaged.

$MA^{(2)}$ – $G_0(k\text{-}q,\omega-\Omega)$, $G_0(k\text{-}q,\omega-2\Omega)$ contributions exact, lines with 3 or more phonons are momentum averaged, etc.

Still can sum all diagrams in the self-energy, calculation still numerically trivial

Define continued fractions: $A_n(\omega) = \dfrac{n g_0(\omega - n\Omega)}{1 - g^2 g_0(\omega - n\Omega) A_{n+1}(\omega)}$

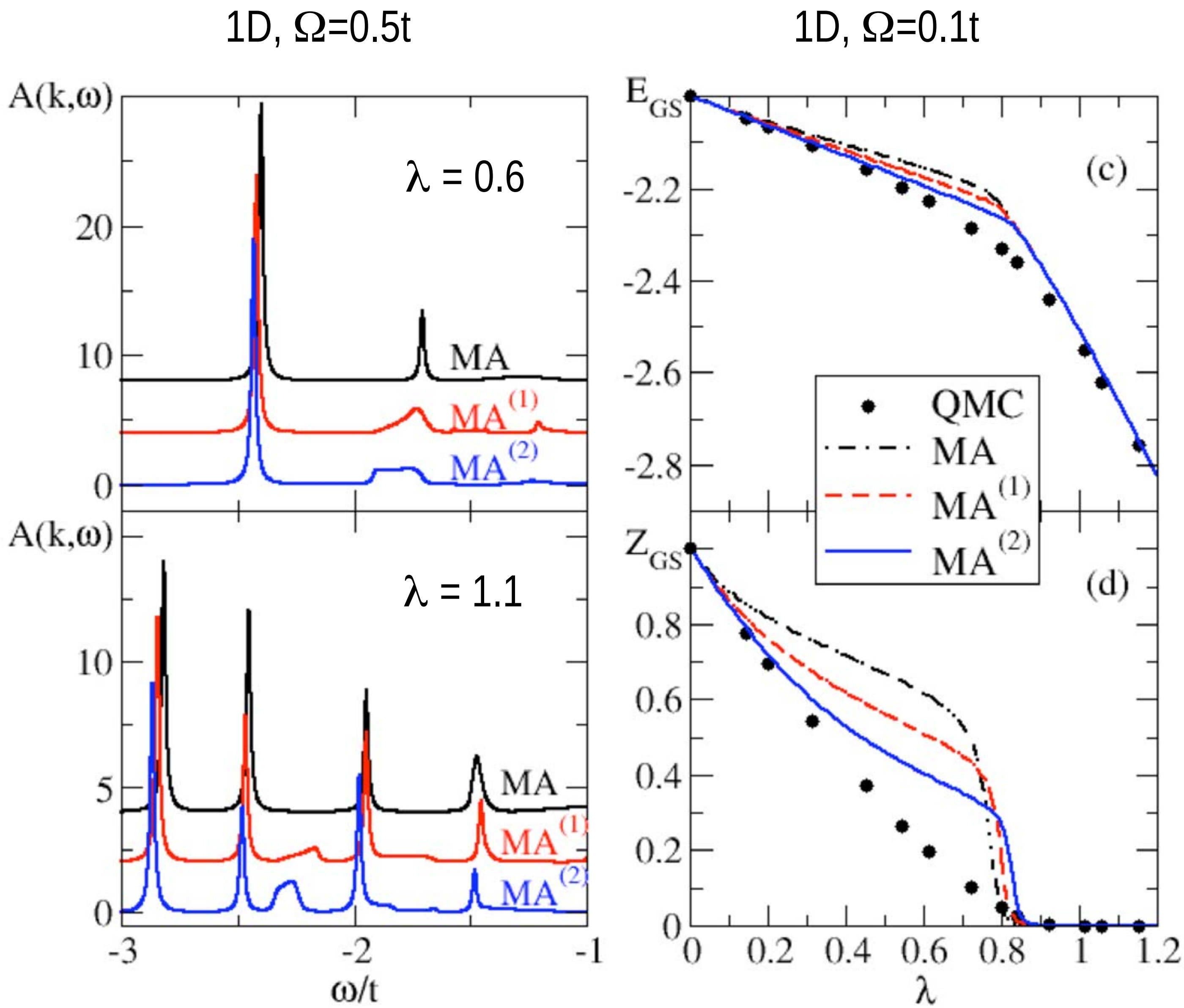
$$\Sigma_{MA^{(0)}}(\omega) = g^2 A_1(\omega)$$

$$\Sigma_{MA^{(1)}}(\omega) = \frac{g^2 g_0(\omega - \Omega - g^2 A_1(\omega - \Omega))}{1 - g^2 g_0(\omega - \Omega - g^2 A_1(\omega - \Omega))\left[A_2(\omega) - A_1(\omega - \Omega)\right]}$$

$\Sigma_{MA^{(2)}}(k,\omega) = \ldots. \;\rightarrow$ acquires explicit momentum dependence

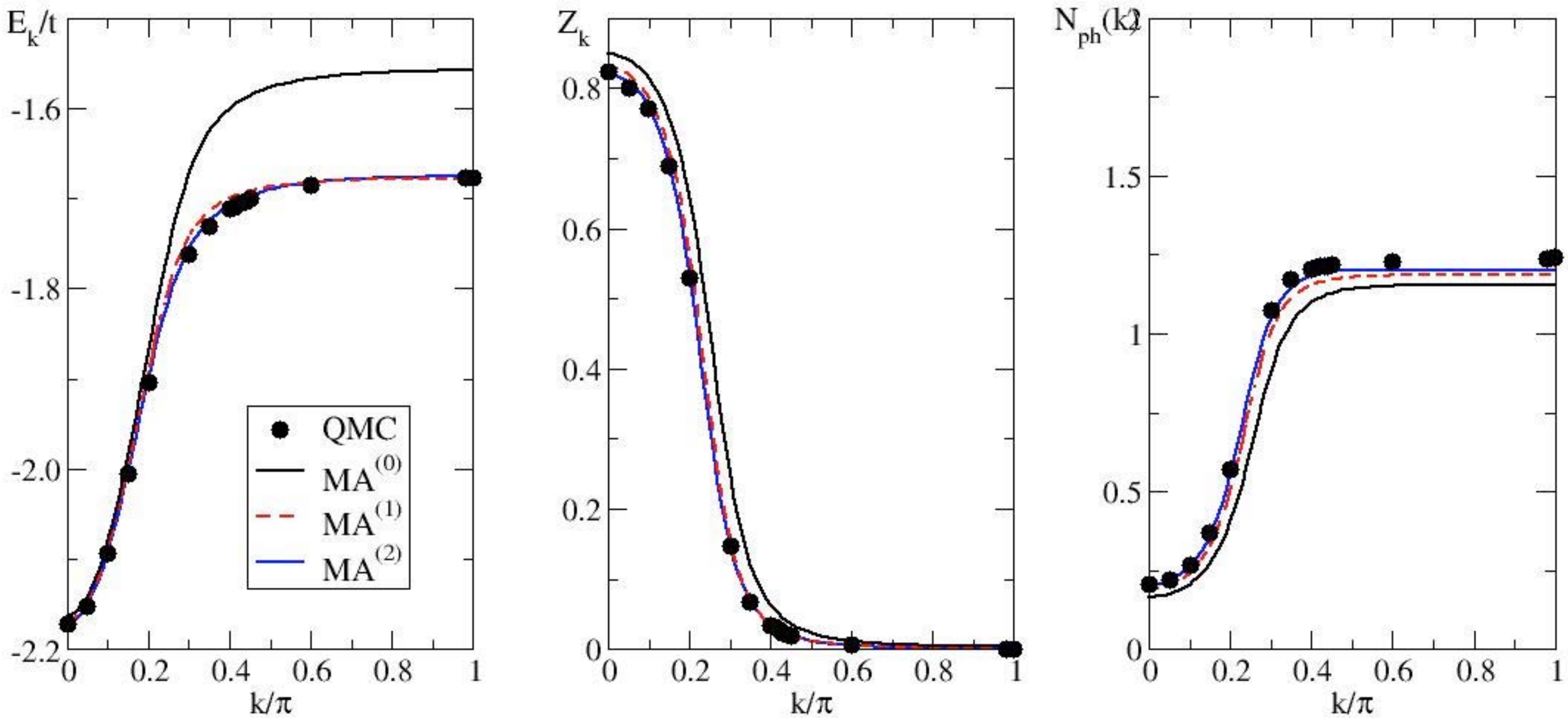
details in M. Berciu and G. Goodvin, PRB 96, 165109 (2007)

(models with g(q) coupling have a k-dependent self-energy from level $MA^{(0)}$)



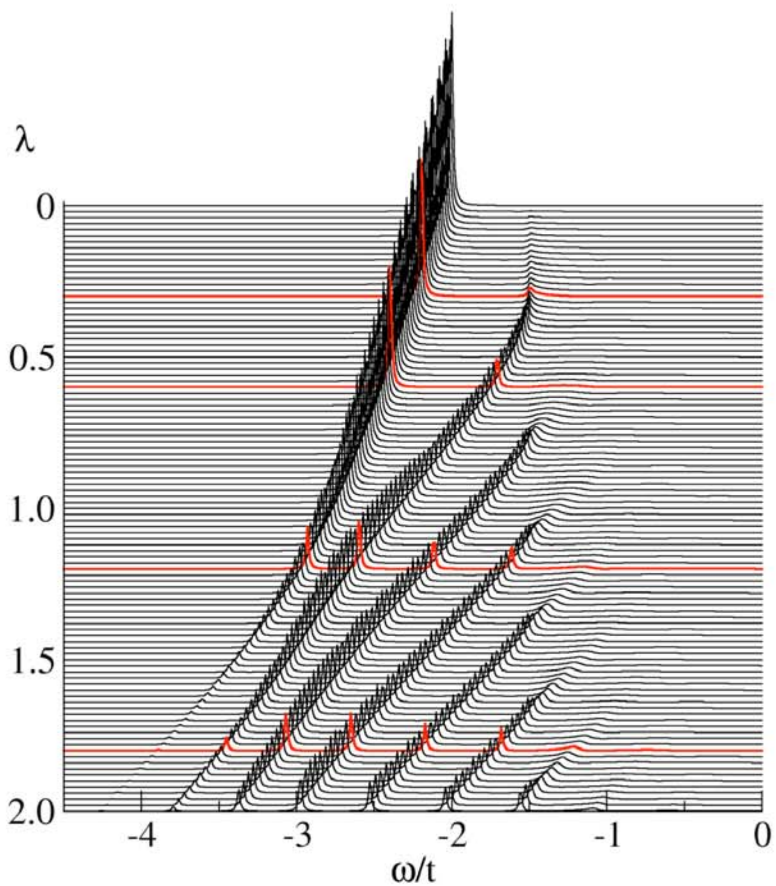
Sum rules:

MA$^{(0)}$ exact up to n=5 and accurate above; MA$^{(1)}$ exact up to n=7 and more accurate above; MA$^{(2)}$ exact up to n=9 and yet more accurate above, …

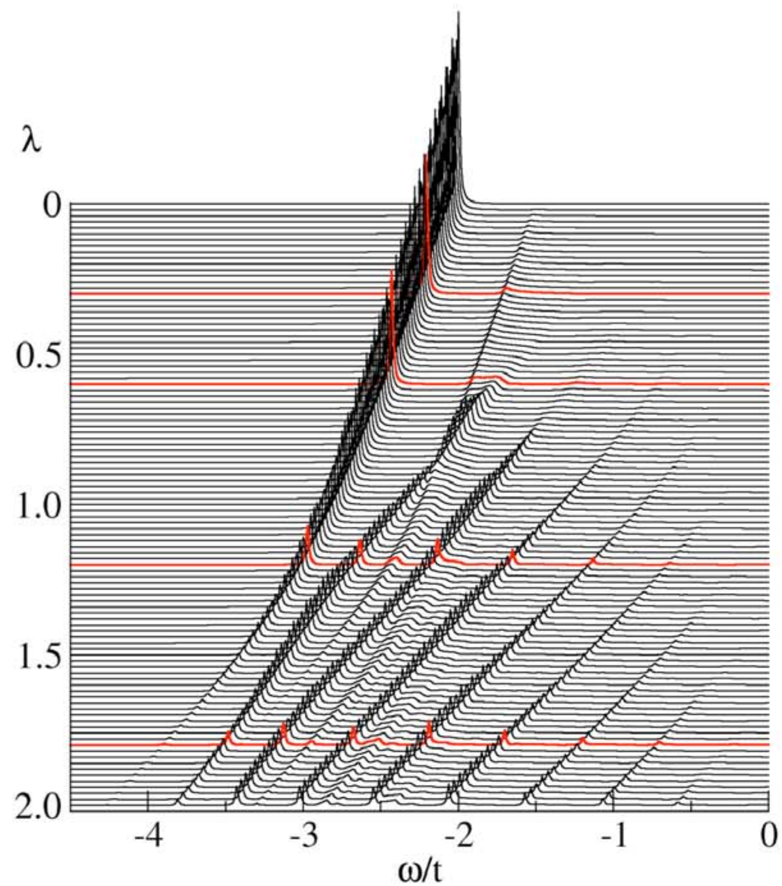


1D, Ω =0.5t, λ =0.25

MA$^{(0)}$



MA$^{(2)}$



(quasi-variational explanation for continuum)

1D, k=0, Ω=0.5t

Conclusions:

→ MA = a hierarchy of approximations providing more and more accurate (but at higher – though still trivial – numerical cost) approximations for the Green's function of a Holstein polaron → proof of principle that such approximations do exist!

→ generalization to multiple phonon modes (**L. Covaci and M. Berciu, EPL 80, 67001 (2007)**)

→ generalizations to electron-phonon models with g(q) coupling: being written up

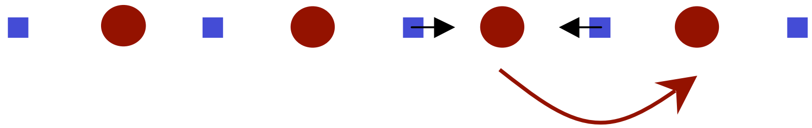
→ generalizations to bi-polarons and hopefully many-electron systems – in progress

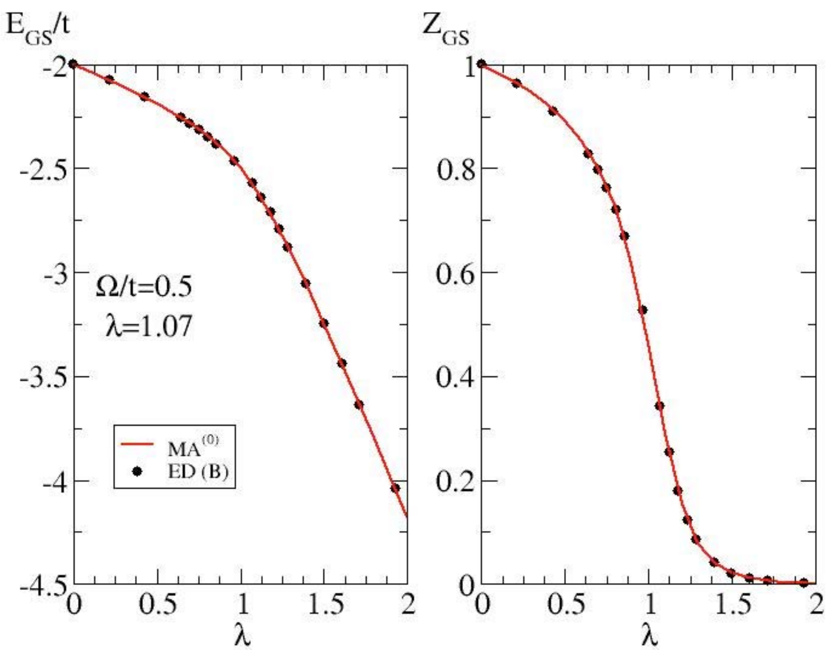
→ generalizations to multiple electron (and phonon) bands (e.g. graphene, spin-orbit coupling, etc) being written up

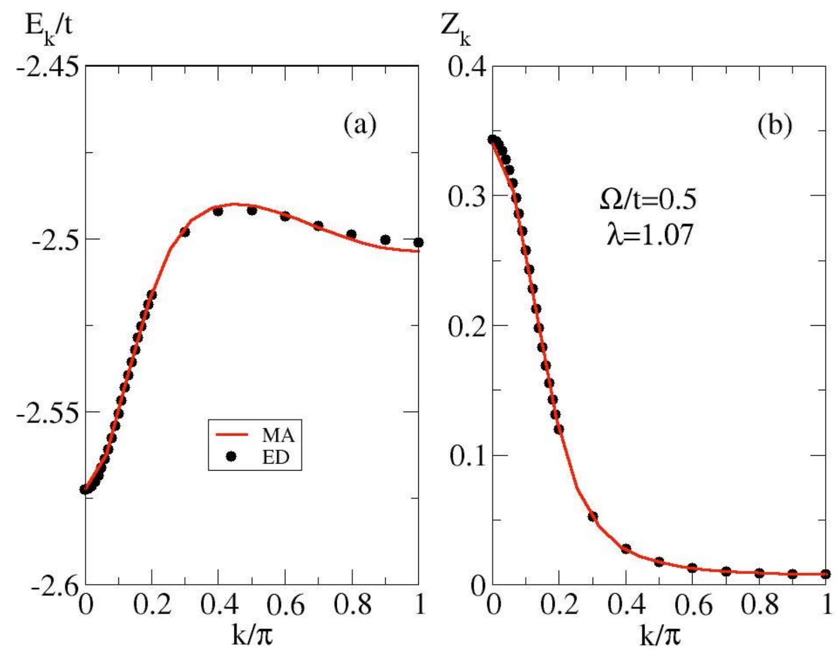
→ combinations …. suggestions for other models coupling fermions to bosons?

→ New strategy to obtain good approximations for intermediary couplings

Coupling to breathing-mode phonon: $g(q) \propto \sin\frac{q}{2}$

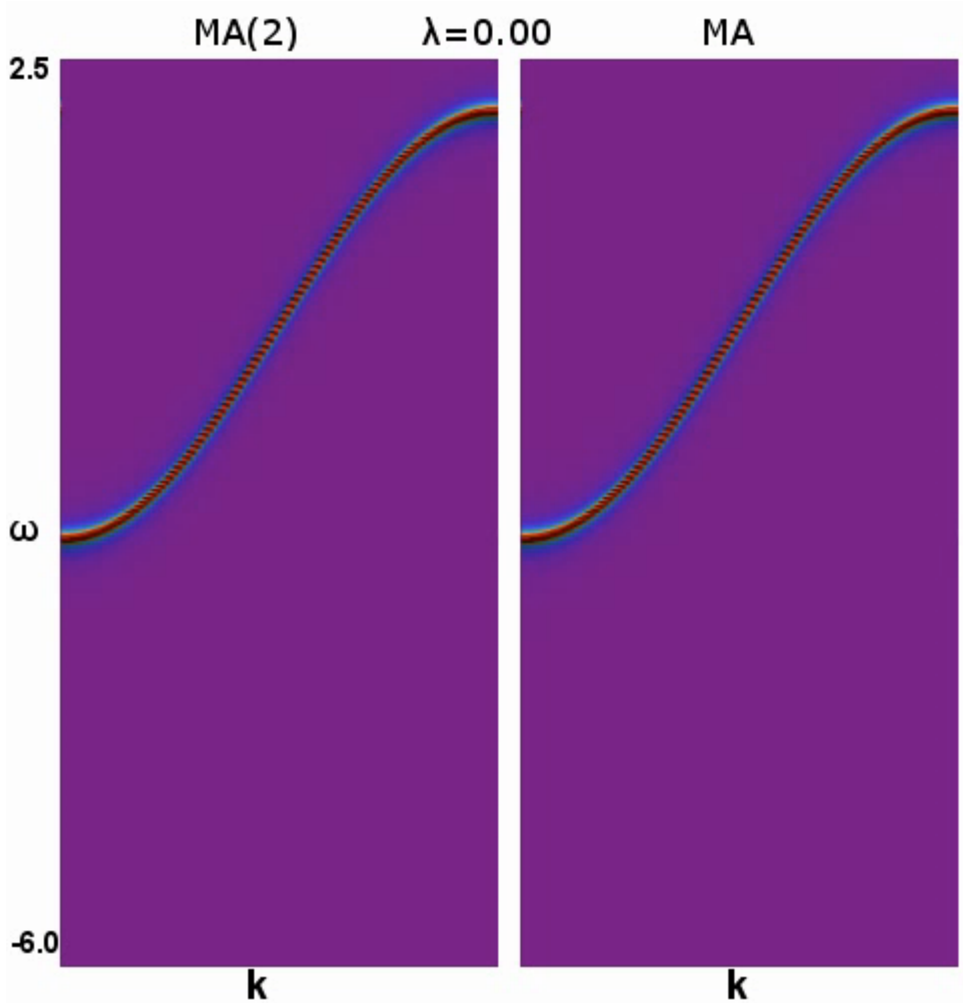






$$E_P(k) \approx t_{1,eff}\cos(ka) + t_{2,eff}\cos(2ka) + \ldots$$

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


MA(2)
λ=0.00
MA
2.5
ω
-6.0
k
k