(about) Polarons

Polaron: if an object (electron, hole, exciton, …) interacts with bosons (phonons, magnons, electron-hole pairs, etc) from its environment and becomes "dressed" by a cloud of such excitations, the composite object is a polaron.

Today: I will only discuss cases with a single polaron in the system (avoids complications regarding polaron-polaron interactions, etc, although of course those are very interesting, too).

Plan: -- quick review of Green's functions (what we want to calculate)

-- a couple of simple examples that can be solved exactly

-- in-depth discussion of the Holstein model

-- some of the many possible generalizations

Quantity of interest: the Green's function or propagator

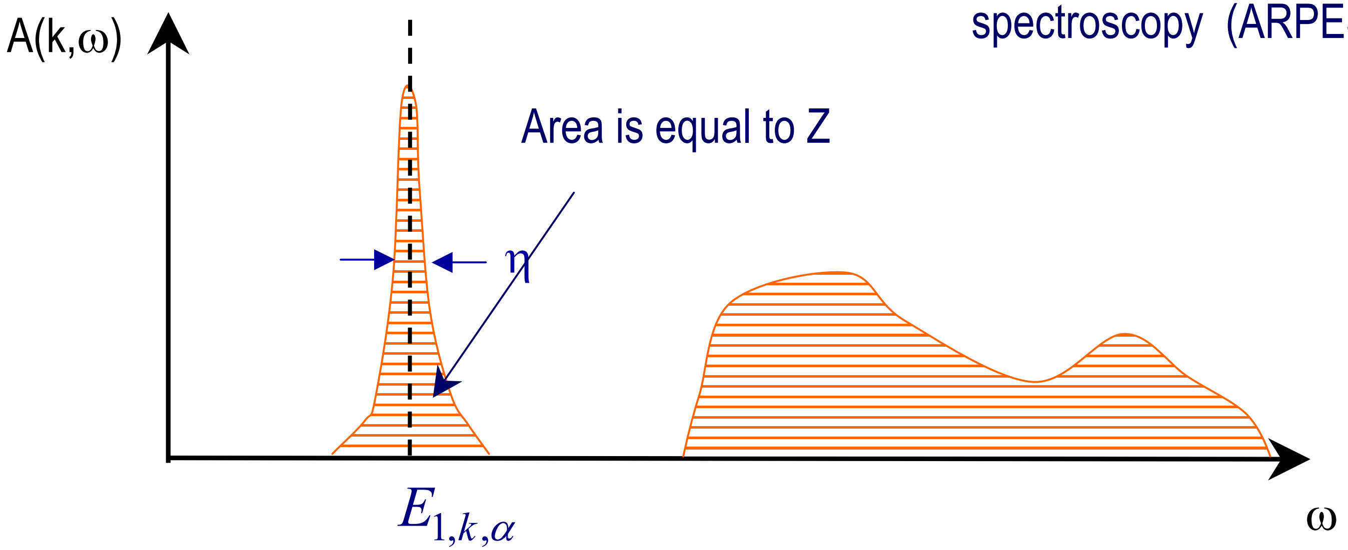
$$H\left|1,k,\alpha\right\rangle = E_{1,k,\alpha}\left|1,k,\alpha\right\rangle$$

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

$$G(k,\omega) \triangleq \left\langle 0\right| c_k \frac{1}{\omega - H + i\eta} c_k^{+}\left|0\right\rangle = \sum_{\alpha} \frac{Z_{1,k,\alpha}}{\omega - E_{1,k,\alpha} + i\eta} \qquad Z_{1,k,\alpha} = \left|\left\langle 1,k,\alpha\right| c_k^{+}\left|0\right\rangle\right|^2$$

$$A(k,\omega) \triangleq -\frac{1}{\pi}\operatorname{Im} G(k,\omega) = \sum_{\alpha} Z_{1,k,\alpha}\,\delta\left(\omega - E_{1,k,\alpha}\right)$$

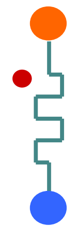
← = spectral weight, is measured (inverse) angle-resolved photoemission spectroscopy (ARPES)



Z = quasiparticle weight → measures how similar is the true wavefunction to a non-interacting (free electron, no bosons) wavefunction

Simplest 1-site model: analog of the Franck-Condon problem

add extra e



= new equilibrium distance

$$h_0 = \frac{\hat{P}^2}{2M} + \frac{M\Omega^2(\hat{X} - X_0)^2}{2} \to \hbar\Omega\left(b^+ b + \frac{1}{2}\right)$$

$$\begin{cases} b = \sqrt{\dfrac{M\Omega}{2\hbar}}\left(\hat{X} - X_0 + i\dfrac{\hat{P}}{M\Omega}\right) \\ b^+ = \sqrt{\dfrac{M\Omega}{2\hbar}}\left(\hat{X} - X_0 - i\dfrac{\hat{P}}{M\Omega}\right) \end{cases} \to \hat{X} - X_0 \propto (b^+ + b)$$

$$h = h_0 + g\hat{n}\hat{X}$$

$$X_0 \to X_0 - \alpha\hat{n}$$

new equilibrium length, determined by how many extra electrons there are

$$h = \Omega b^\dagger b + g\hat{n}(b^\dagger + b) \to \Omega b^\dagger b + g(b^\dagger + b) = \Omega B^\dagger B - \frac{g^2}{\Omega}$$

If we're adding one electron

$$B = b + \frac{g}{\Omega} \to \left[B, B^\dagger\right] = \left[b, b^\dagger\right] = 1$$

Ground-state is: $\left|GS\right\rangle = c^\dagger \left|-\frac{g}{\Omega}\right\rangle \to E_{GS} = -\frac{g^2}{\Omega}; \left\langle b^\dagger b\right\rangle = \frac{g^2}{\Omega^2}$

where $b\left|-\frac{g}{\Omega}\right\rangle = -\frac{g}{\Omega}\left|-\frac{g}{\Omega}\right\rangle \to B\left|-\frac{g}{\Omega}\right\rangle = 0$

while excited states have energies $\mathrm{E_n} = -\frac{g^2}{\Omega} + n\Omega$

and eigenfunctions of the general form: $c^\dagger \frac{B^{\dagger n}}{\sqrt{n!}}\left|-\frac{g}{\Omega}\right\rangle$

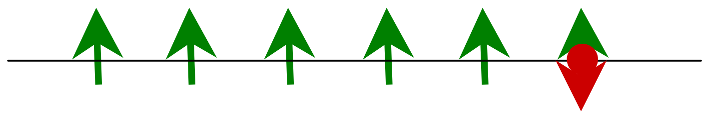
Side-note: coherent states properties in the homework

$$b\left|\alpha\right\rangle = \alpha\left|\alpha\right\rangle \to \left|\alpha\right\rangle = e^{-\frac{|\alpha|^2}{2} + \alpha b^\dagger}\left|0\right\rangle$$

Green's function can be calculated since eigenspectrum is known → homework

Spin-polaron → electron in a 1D FM lattice of spins ½ (many generalizations possible)

see references in M. Berciu and G. A. Sawatzky, PRB 79, 195116 (2009)



$$H=-J\sum_i\left(\vec{S}_i\vec{S}_{i+1}-\frac{1}{4}\right)-t\sum_{i,\sigma}\left(c_{i,\sigma}^\dagger c_{i+1,\sigma}+h.c.\right)+J_0\sum_i\vec{s}_i\vec{S}_i$$

If the electron is spin up → boring (no spin flip possible, energy of electron just shifted by const)

Introduce electron with spin-down → can calculate exactly its Green's function:

$$G(k,\omega)=\left\langle FM\left|c_{k\downarrow}\hat{G}(\omega)c_{k\downarrow}^\dagger\right|FM\right\rangle$$

because the electron can flip at most once, creating a magnon in the process. Because the Hilbert space is still rather small, problem can be solved exactly (see references).

Strong coupling limit: $J_0 >> t, J$

First, find eigenstate of largest term → if the electron is at site i then it locks into a singlet with the spin at that site. The energy of the singlet is $-3J_0/4$.

This describes the polaron structure in this limit: 50% chance for spin-down electron, 50% chance of spin-up electron and flipped lattice spin (=magnon bound to the electron)

To find the dispersion, make a plane-wave of momentum k from these states:

$$|P,k\rangle = \frac{1}{\sqrt{N}} \sum_i e^{ikR_i} \frac{c_{i\uparrow}^\dagger S_i^- - c_{i\downarrow}^\dagger}{\sqrt{2}} |FM\rangle$$

$$E_P(k) = -\frac{3}{4}J_0 + \langle P,k|\hat{T} + \hat{H}_{FM}|P,k\rangle = -\frac{3}{4}J_0 - 2t^* \cos(ka) + const.$$

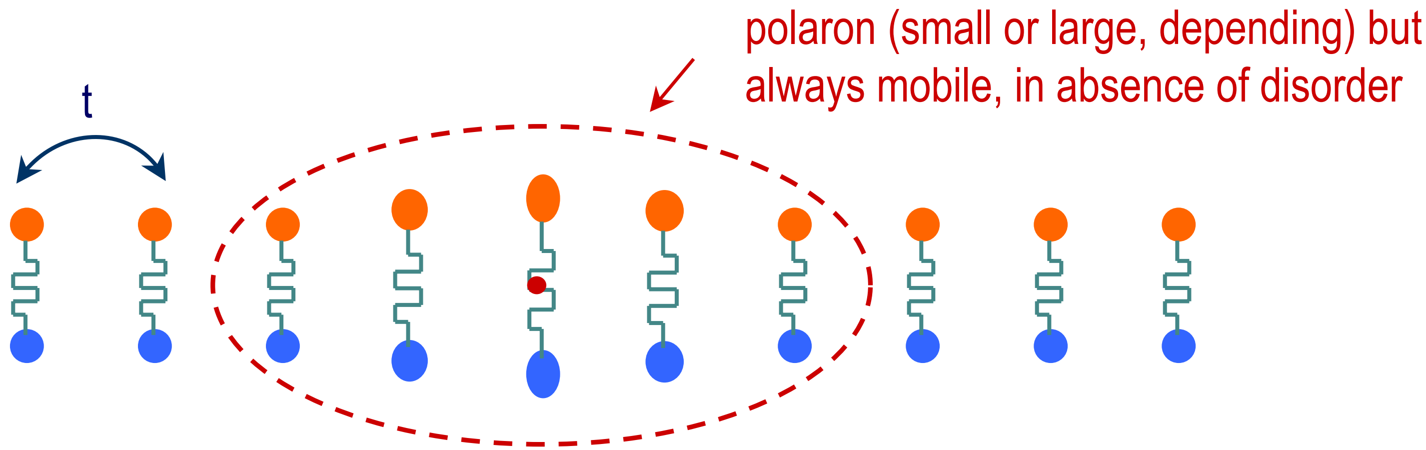
Polaron hopping $t^*=t/2$ → polaron is precisely twice as heavy as free particle. This is because the "cloud overlap" is exactly 50% in this limit (homework).

Such exact solutions on a lattice are very rare. In fact, as far as I know, this is the only kind of model that admits such an exact solution.

Polaron (lattice polaron) = electron + lattice distortion (phonon cloud) surrounding it

→ very old problem: Landau, 1933;

→ most studied lattice model = Holstein model (not very realistic)



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

3 energy scales: t, Ω, g → 2 dimensionless parameters $\lambda = g^2/(2dt\Omega)$, Ω/t (d is lattice dimension)

Eigenstates are linear combinations of states with the electron at different sites, surrounded by a lattice distortion (cloud of phonons). Can have any number of phonons → problem cannot be solved exactly for arbitrary t, g, Ω.

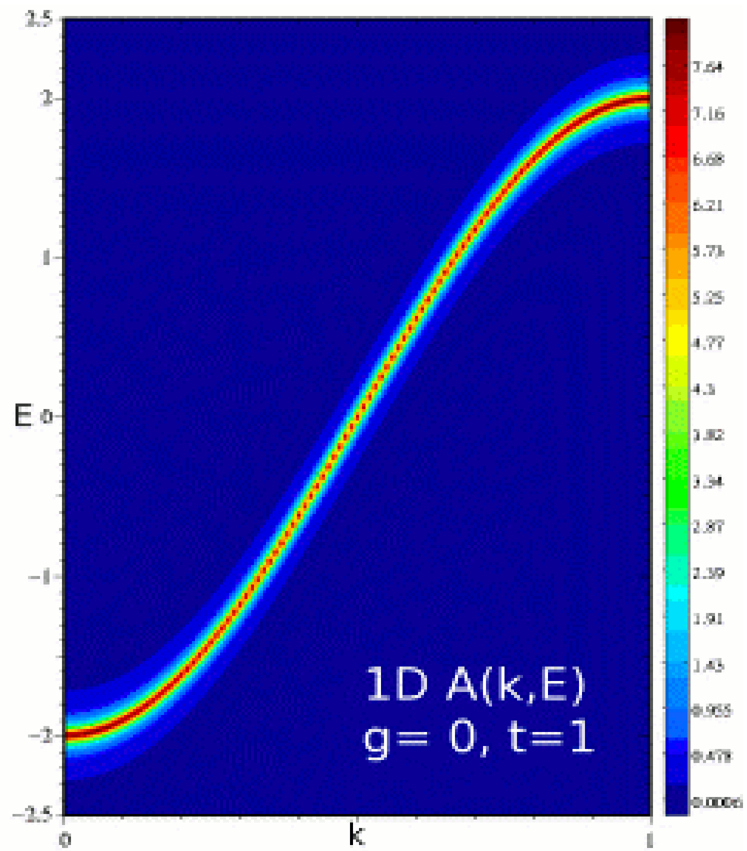
weak coupling $\lambda = \frac{g^2}{2dt\Omega} = 0 \quad (g = 0)$

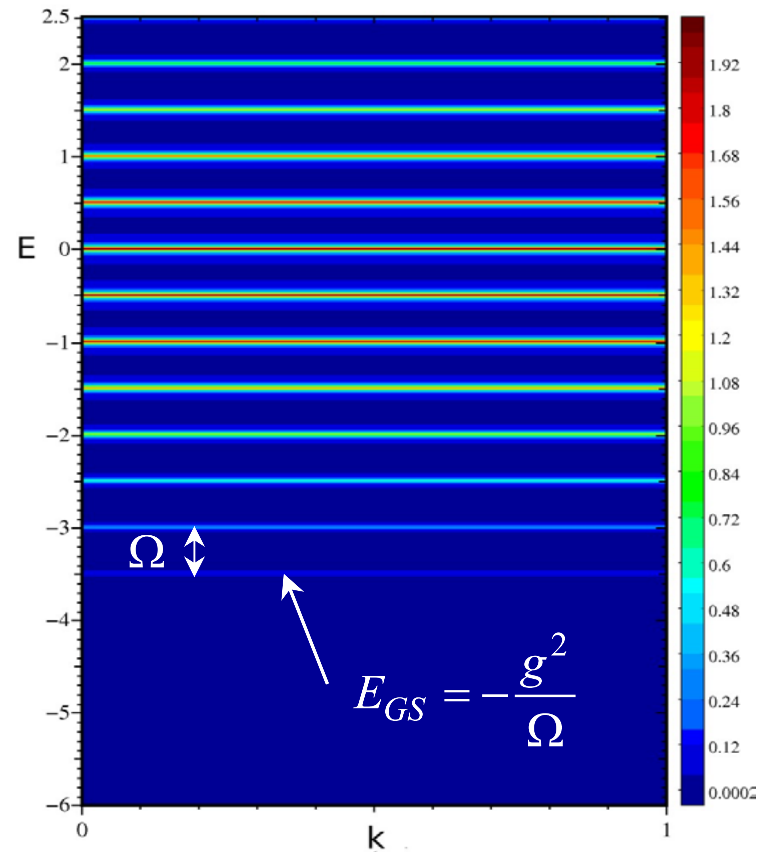
Lang-Firsov impurity limit $\lambda = \frac{g^2}{2dt\Omega} = \infty \quad (t = 0)$

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

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

$$E_n = -\frac{g^2}{\Omega} + n\Omega$$





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

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

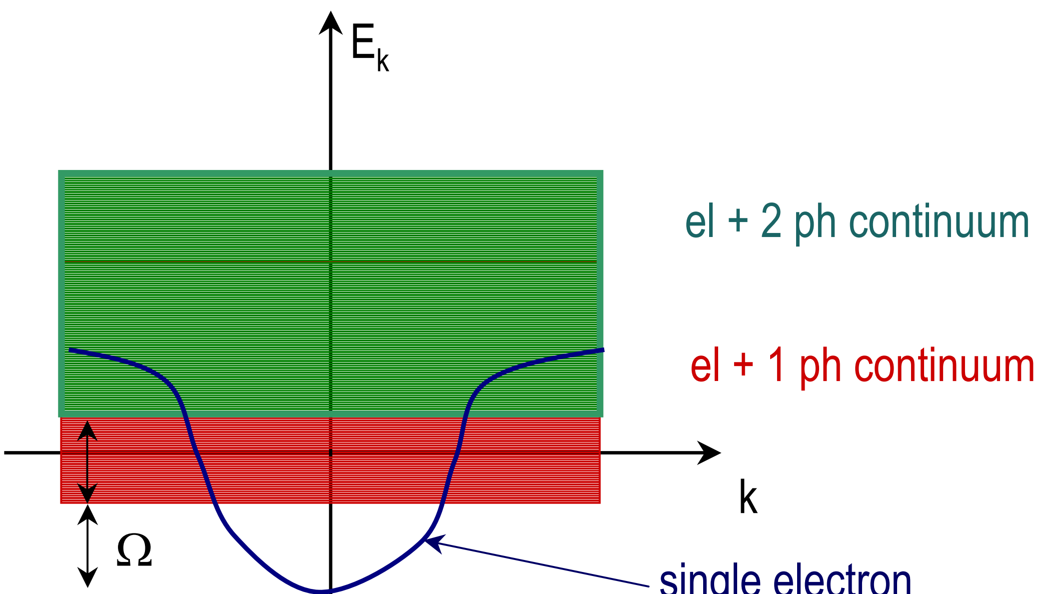
$$= \sum_{\vec{k}} \varepsilon_{\vec{k}} c_{\vec{k}}^{+} c_{\vec{k}} + \Omega\sum_{\vec{q}} b_{\vec{q}}^{+} b_{\vec{q}} + \frac{g}{\sqrt{N}}\sum_{\vec{k},\vec{q}} c_{\vec{k}-\vec{q}}^{+} c_{\vec{k}}\left(b_{\vec{q}}^{+} + b_{-\vec{q}}\right)$$

(spin is irrelevant, N = number of unit cells, → infinity at the end, all k,q-sums over Brillouin zone)

Asymptotic behavior:

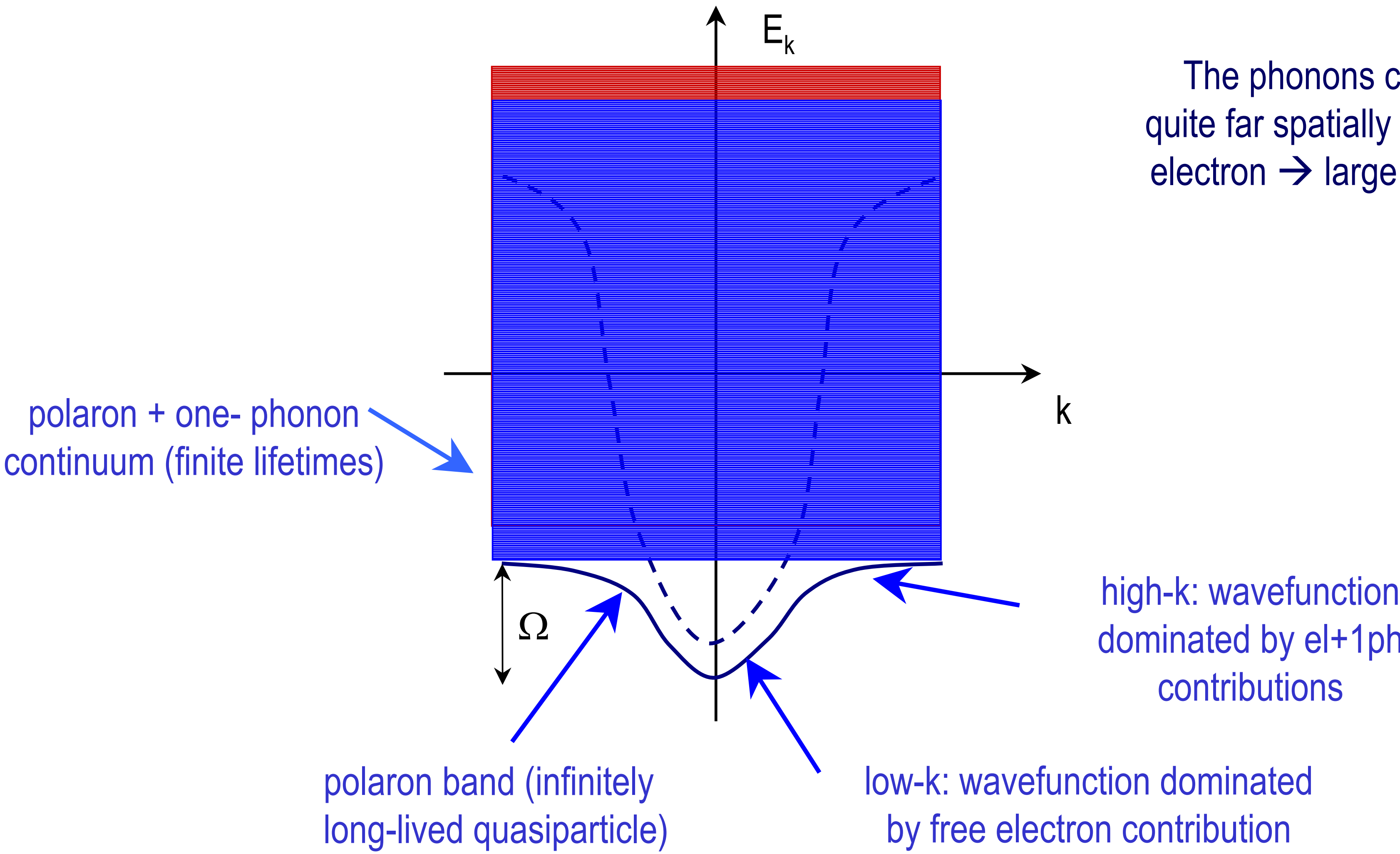
→ zero-coupling limit, g=0 → eigenstates of given k: $c_{\vec{k}}^{+}|0\rangle,\ c_{\vec{k}-\vec{q}}^{+}b_{\vec{q}}^{+}|0\rangle,\ c_{\vec{k}-\vec{q}-\vec{q}'}^{+}b_{\vec{q}}^{+}b_{\vec{q}'}^{+}|0\rangle, \dots$

with eigenenergies $\varepsilon_{\vec{k}},\ \varepsilon_{\vec{k}-\vec{q}} + \Omega,\ \varepsilon_{\vec{k}-\vec{q}-\vec{q}'} + 2\Omega, \dots$ where, for example, $\varepsilon_{\vec{k}} = -2t\sum_{i=1}^{d}\cos k_i$



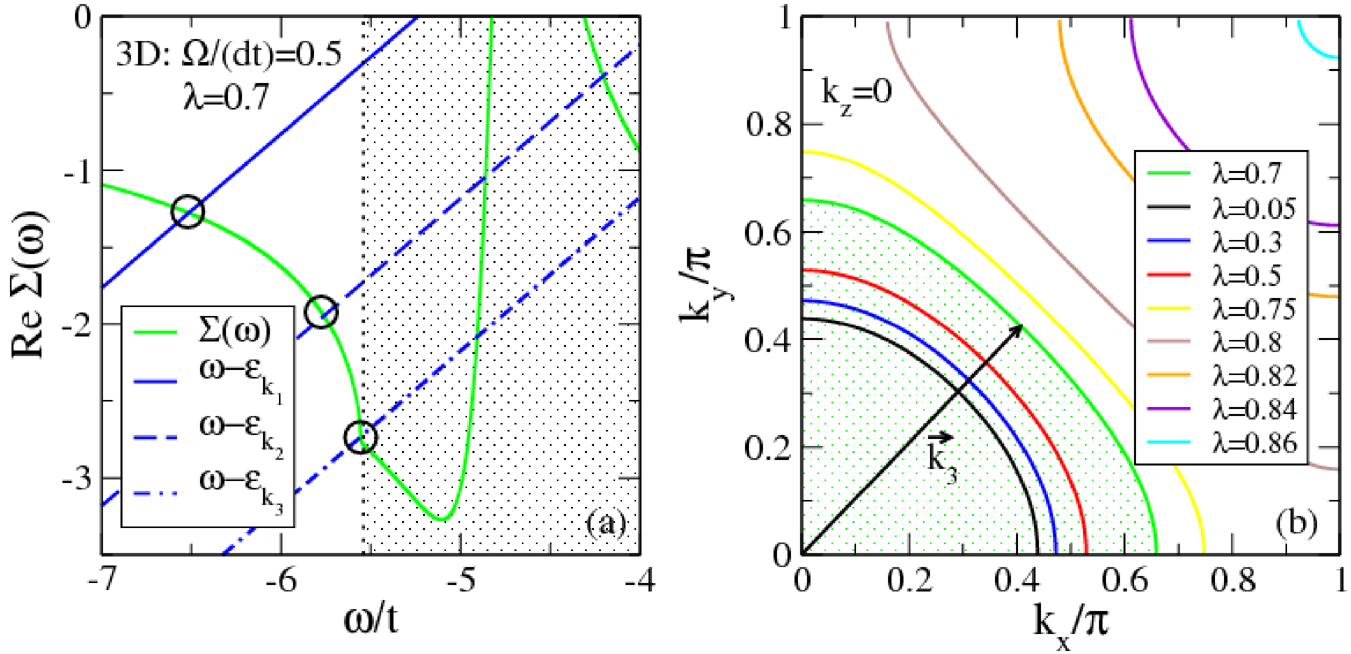
→ weak coupling, g = "small" → low-energy eigenstates of known k: $\left|\psi_{\vec{k}}\right\rangle = c_{\vec{k}}^{+}\left|0\right\rangle + \sum_{\vec{q}} \phi_{\vec{q}} c_{\vec{k}-\vec{q}}^{+} b_{\vec{q}}^{+}\left|0\right\rangle$

with eigenenergies $E_{\vec{k}} = \varepsilon_{\vec{k}} - \frac{1}{N}\sum_{\vec{q}} \frac{g^2}{\left(\Omega + \varepsilon_{\vec{k}-\vec{q}}\right) - \varepsilon_{\vec{k}}} + \ldots$ (for k< k_{cross})



The phonons can be quite far spatially from the electron → large polaron

In fact, a polaron state exists everywhere in the BZ only in d=1,2. In d=3 and weak coupling, the polaron exists only near the center of the BZ.



$$G(k,\omega)=\frac{1}{\omega-\varepsilon_k-\Sigma(k,\omega)+i\eta}\rightarrow\omega-\varepsilon_k=\mathrm{Re}[\Sigma(\omega)];\quad \mathrm{Im}[\Sigma(\omega)]=0$$

G.L. Goodvin and M. Berciu, EuroPhys. Lett. 92, 37006 (2010)

→ very strong coupling, λ>>1 (t→ 0) →small polaron energy is

$$E_k = -\frac{g^2}{\Omega} + e^{-\frac{g^2}{\Omega^2}}\varepsilon_k + \ldots \rightarrow t_{eff} = te^{-\frac{g^2}{\Omega^2}} \rightarrow m_{eff} = me^{\frac{g^2}{\Omega^2}}$$

$$\text{and wavefunction is } \left|\psi_k\right\rangle = \sum_i \frac{e^{i\vec{k}\cdot\vec{R}_i}}{\sqrt{N}} c_i^\dagger \left|-\frac{g}{\Omega}\right\rangle_i$$

Again, must have a polaron+one-phonon continuum at $E_{GS} + \Omega$ → details too nasty

Because here polaron dispersion is so flat, there is a polaron state everywhere in the BZ.

- Diagrammatic Quantum Monte Carlo (Prokof'ev, Svistunov and co-workers)

→calculate Green's function in imaginary time

$$G(k,\tau) = \langle 0 | c_k e^{-\tau H} c_k^\dagger | 0 \rangle = \sum_\alpha e^{-\tau E_{1,k,\alpha}} \left| \langle 1,k,\alpha | c_k^\dagger | 0 \rangle \right|^2 \xrightarrow[\tau \to \infty]{} Z_k e^{-\tau E_k}$$

Basically, use Metropolis algorithm to sample which diagrams to sum, and keep summing numerically until convergence is reached

- Quantum Monte Carlo methods (Kornilovitch in Alexandrov group, Hohenadler in Fehske group, …) → write partition function as path integral, use Trotter to discretize it, then evaluate. Mostly low-energy properties are calculated/shown.

- Exact diagonalization = ED → finite system (still need to truncate Hilbert space) → can get whole spectrum and then build G(k,w)

- Variational methods

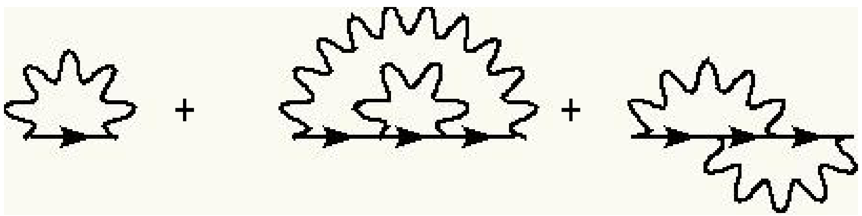
- Cluster perturbation theory: ED finite system, then use perturbation in hopping to "sew" finite pieces together → infinite system.

- + 1D, DMRG+DMFT

→…. (lots of work done in these 50 years, as you may imagine)

Analytic approaches (other than perturbation theory) → calculate self-energy

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

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

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).

MA also has variational meaning:

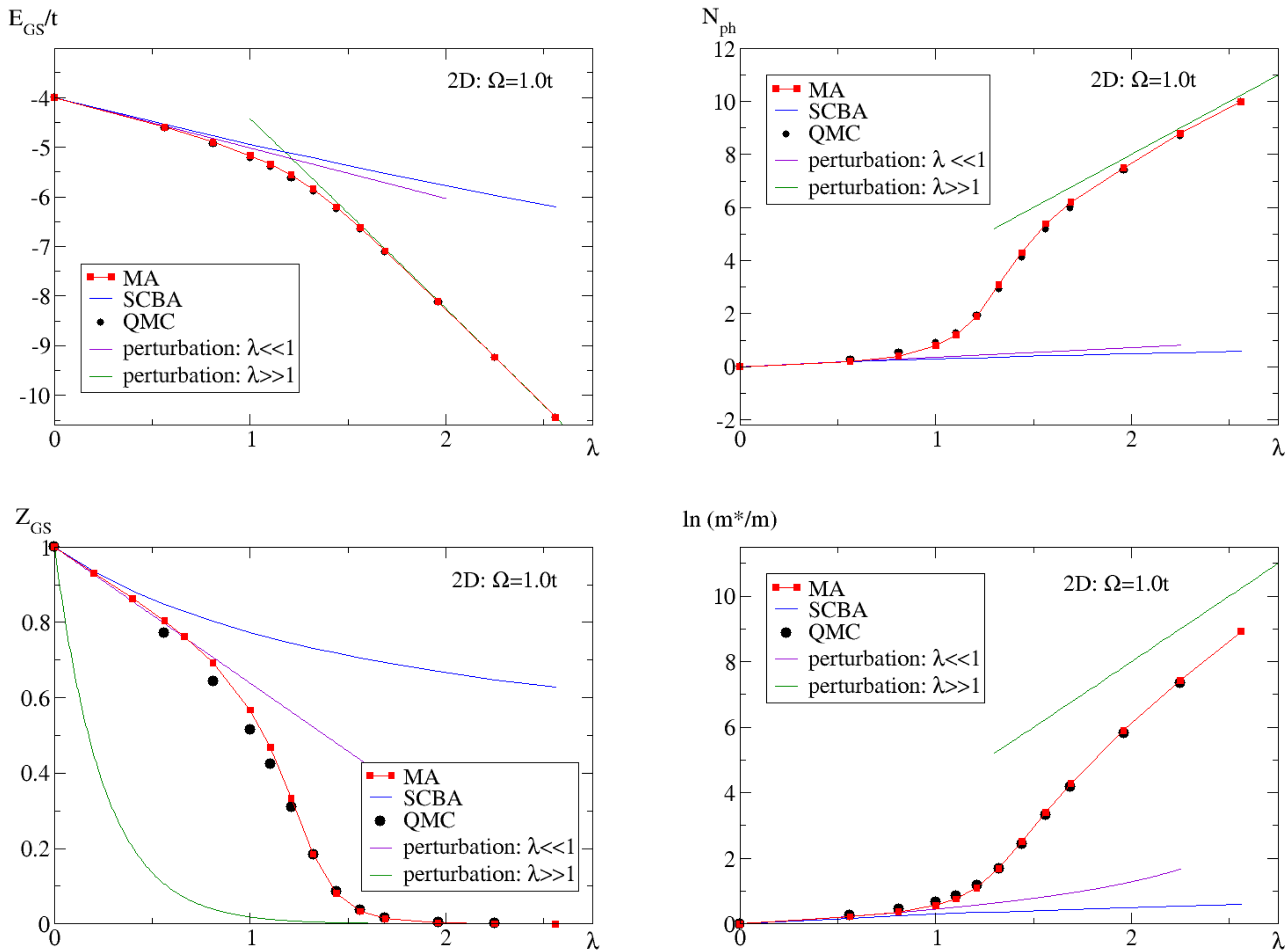
→ only certain kinds of bosonic clouds allowed (**O. S. Barišic, PRL 98, 209701 (2007)**)

→ what is reasonable depends on the model. In the simplest case (Holstein model):

$$\mathrm{MA}^{(0)} \to c_i^\dagger \left(b_j^\dagger\right)^n |0\rangle, \quad (\forall) i, j, n$$

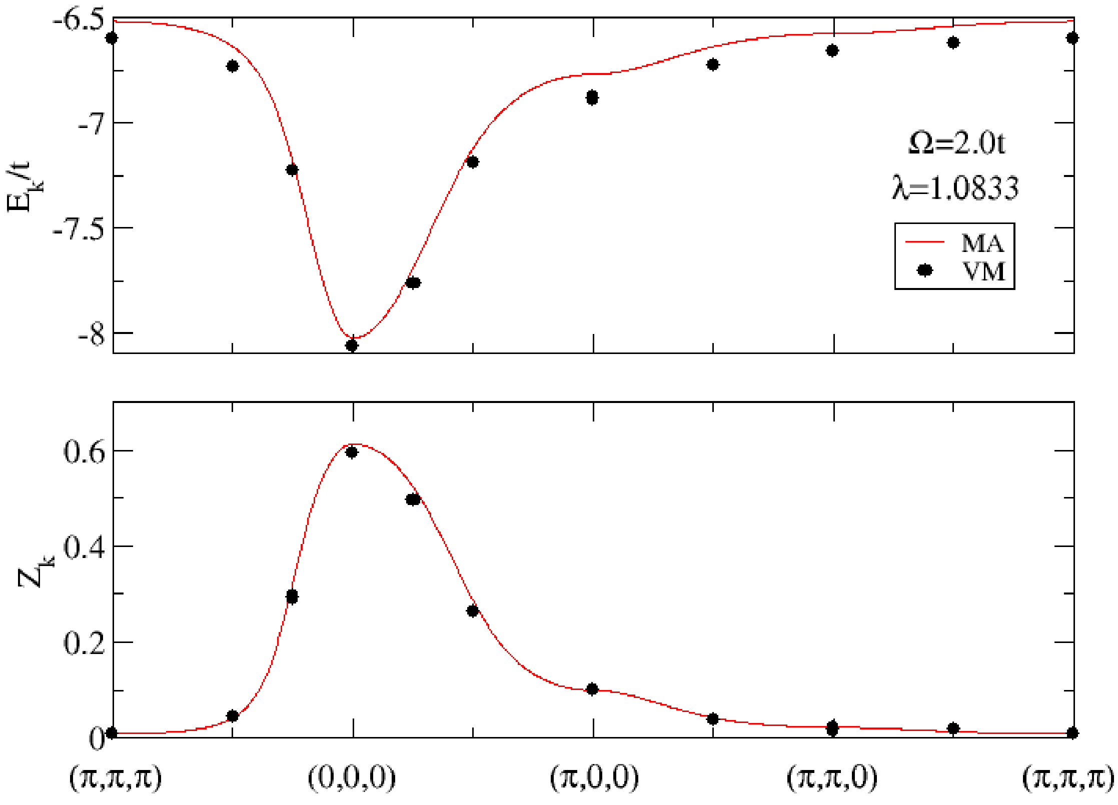
$$\mathrm{MA}^{(1)} \to c_i^\dagger \left(b_j^\dagger\right)^n b_l^\dagger |0\rangle, \quad (\forall) i, j, l, n$$

(needed to describe polaron + one-boson continuum)



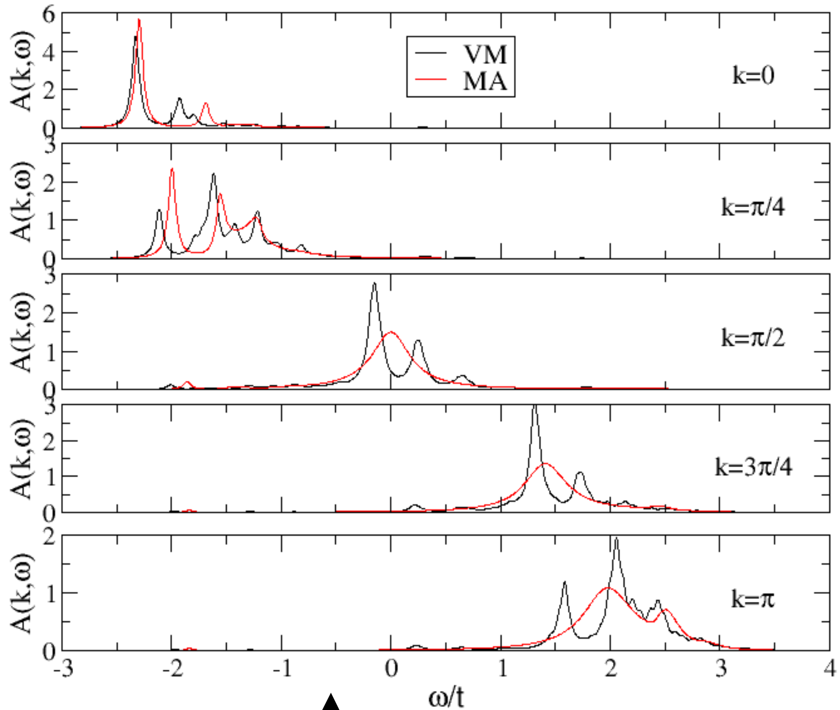
E_{GS}/t
2D: Ω=1.0t
MA
SCBA
QMC
perturbation: λ<<1
perturbation: λ>>1
λ
N_{ph}
2D: Ω=1.0t
MA
SCBA
QMC
perturbation: λ <<1
perturbation: λ>>1
λ
Z_{GS}
2D: Ω=1.0t
MA
SCBA
QMC
perturbation: λ<<1
perturbation: λ>>1
λ
ln (m*/m)
2D: Ω=1.0t
MA
SCBA
QMC
perturbation: λ<<1
perturbation: λ>>1
λ

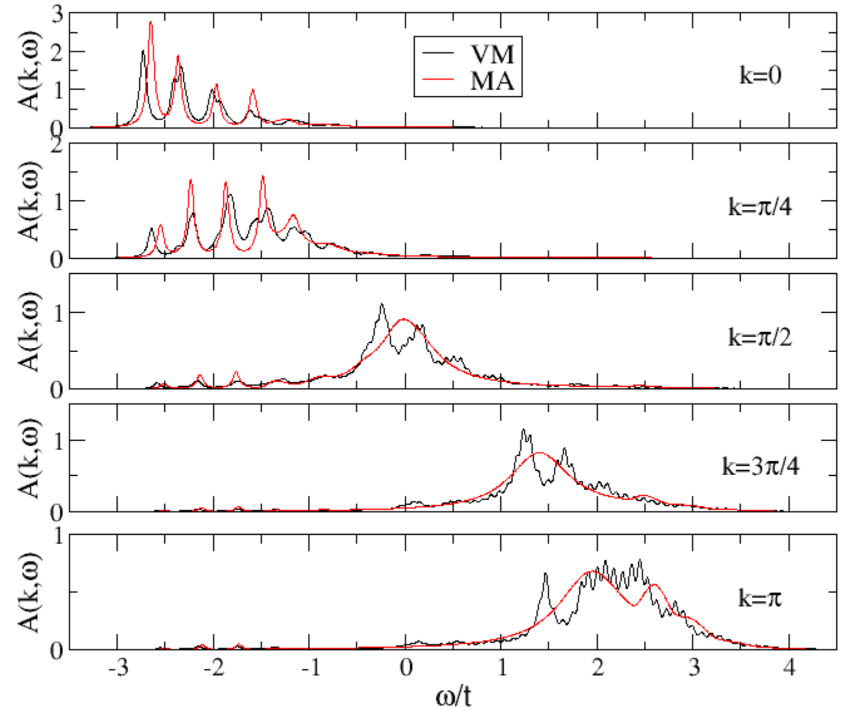
3D Polaron dispersion



Polaron bandwidth much narrower than 12t !

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

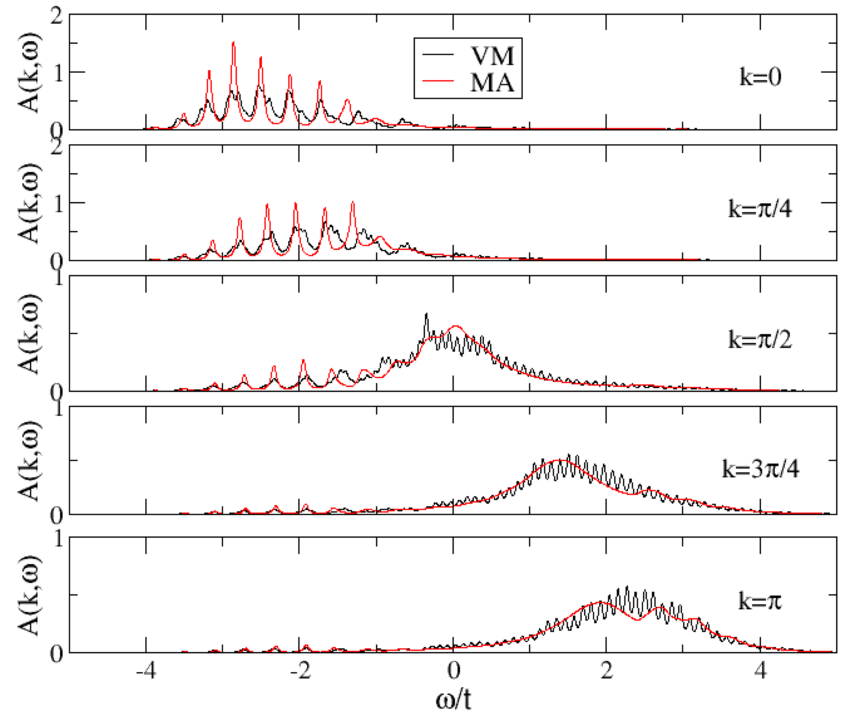




$\lambda = 0.5$

$\lambda = 1$

$\lambda = 2$



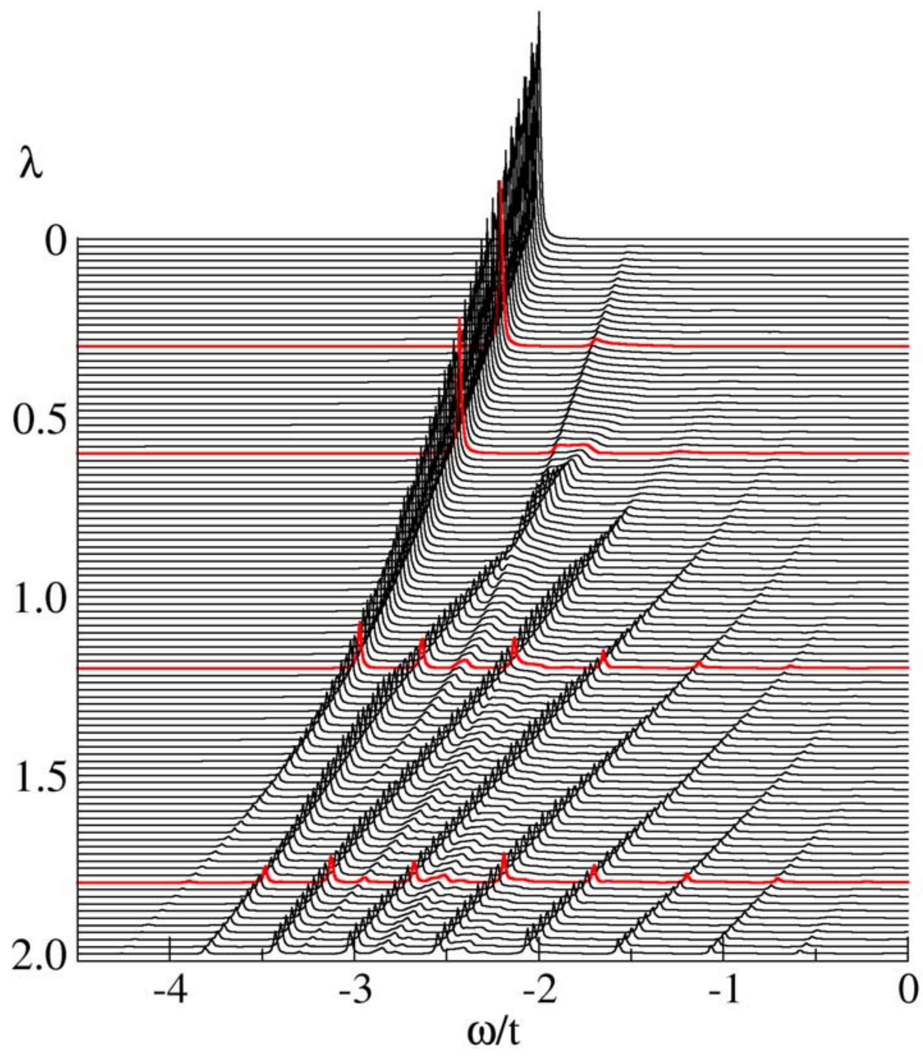
A(k,ω) in 1D, Ω =0.4 t

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

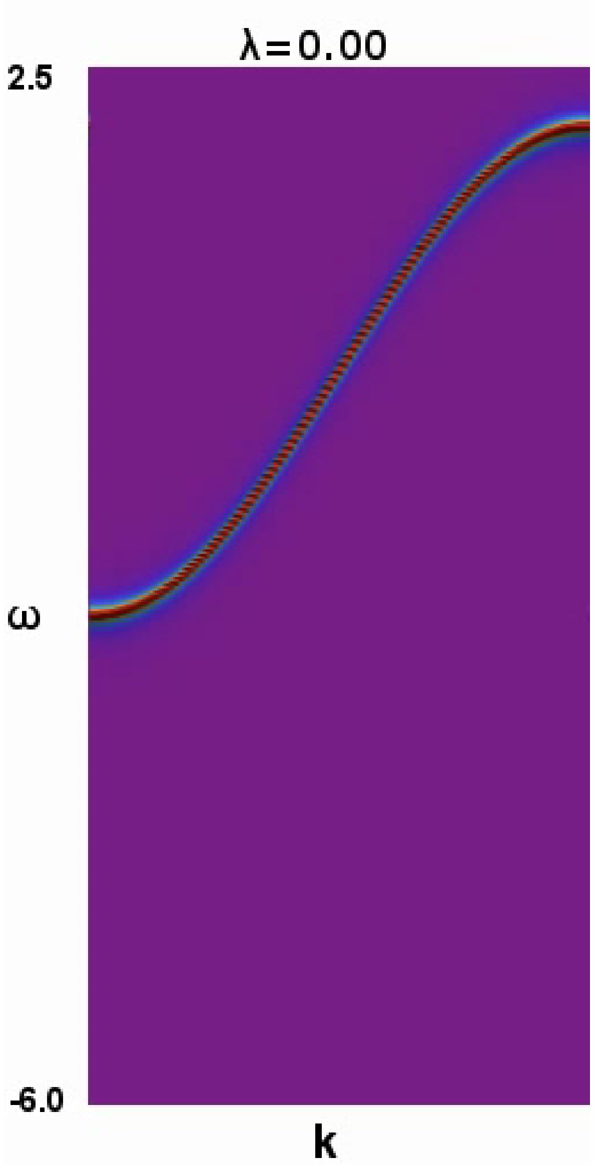
MA becomes exact for small, large λ

MA$^{(2)}$

1D, k=0, Ω=0.5t

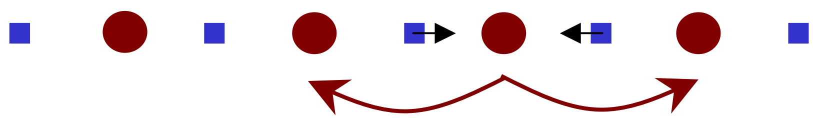


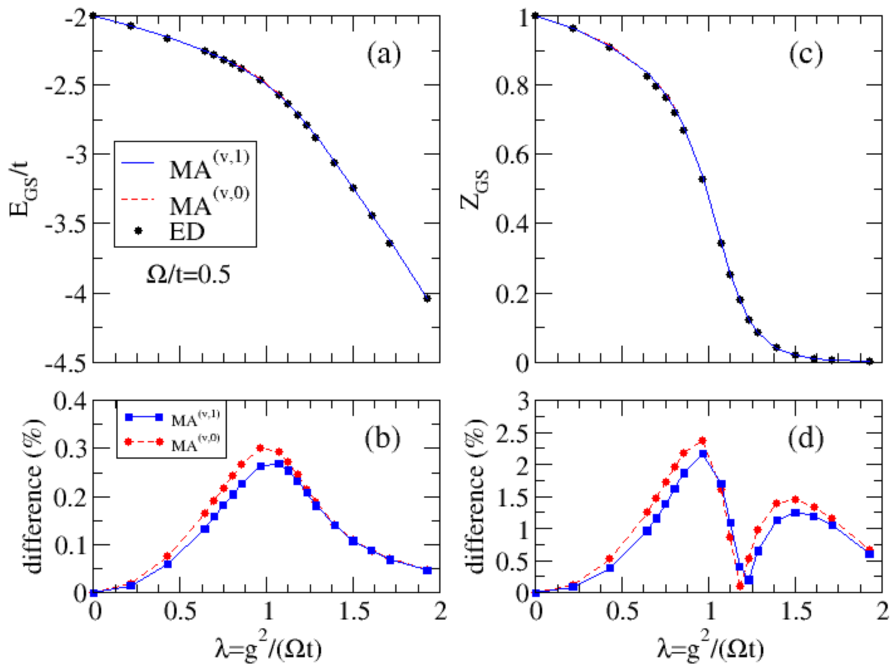
Our answer to how spectral weight evolves as λ increases from weak to strong coupling

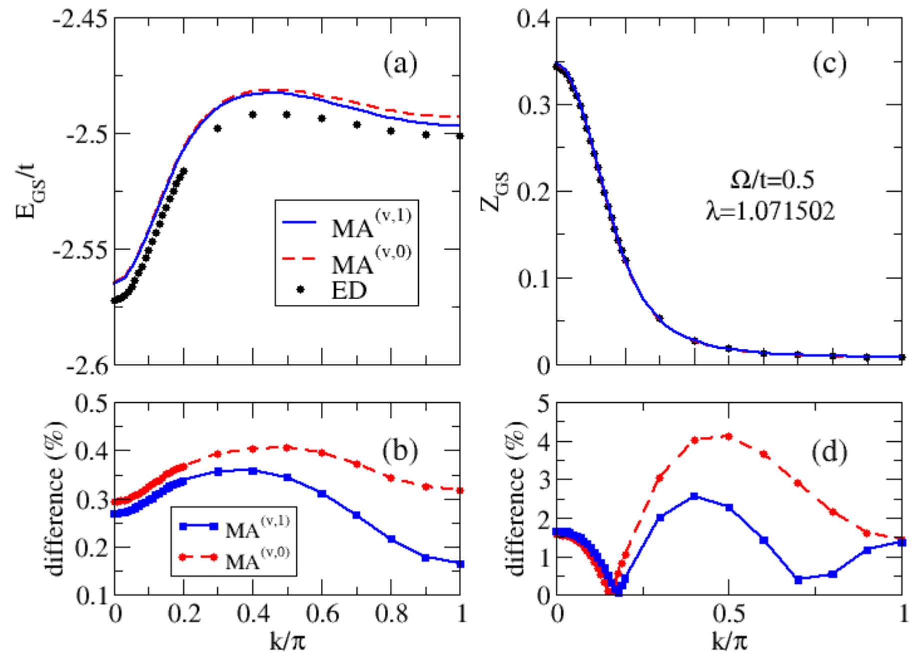


Away from Holstein:

Coupling to breathing-mode phonon: $g(q) \propto i \sin\frac{q}{2}$:scattering amplitude depends on bosons's momentum.







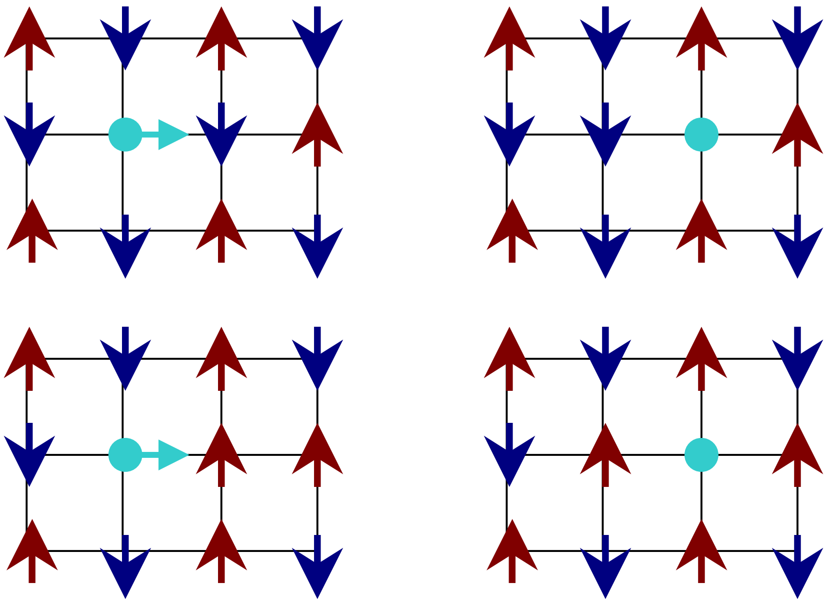
G. L. Goodvin and M. Berciu, PRB 78, 235120 (2008)

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

Phonons can also modulate the hopping integral!

Model 1: Edwards model (A. Alvermann, D.M. Edwards and H. Fehske, PRL 98, 056602 (2007))

Example (not 100% accurate) consider particle moving in an AFM Ising background.



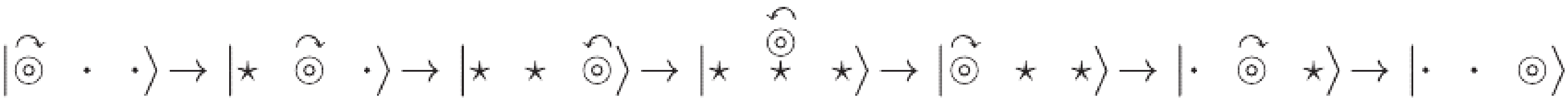
← boson (= magnon) created at initial site

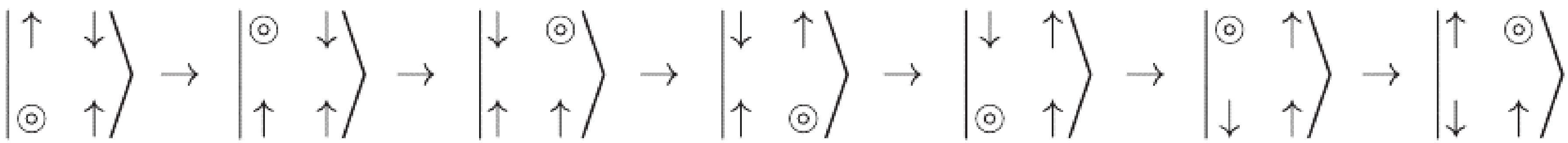
← or boson annihilated at final site

$$H = -t_b \sum_{i,j} c_j^\dagger c_i (b_j + b_i^\dagger) + \Omega \sum_i b_i^\dagger b_i + \lambda \sum_i \left(b_i^\dagger + b_i \right) \rightarrow$$

$$H = -t_f \sum_{i,j} c_j^\dagger c_i - t_b \sum_{i,j} c_j^\dagger c_i (b_j + b_i^\dagger) + \Omega \sum_i b_i^\dagger b_i \quad \text{where } t_f = 2t_b \frac{\lambda}{\Omega}$$

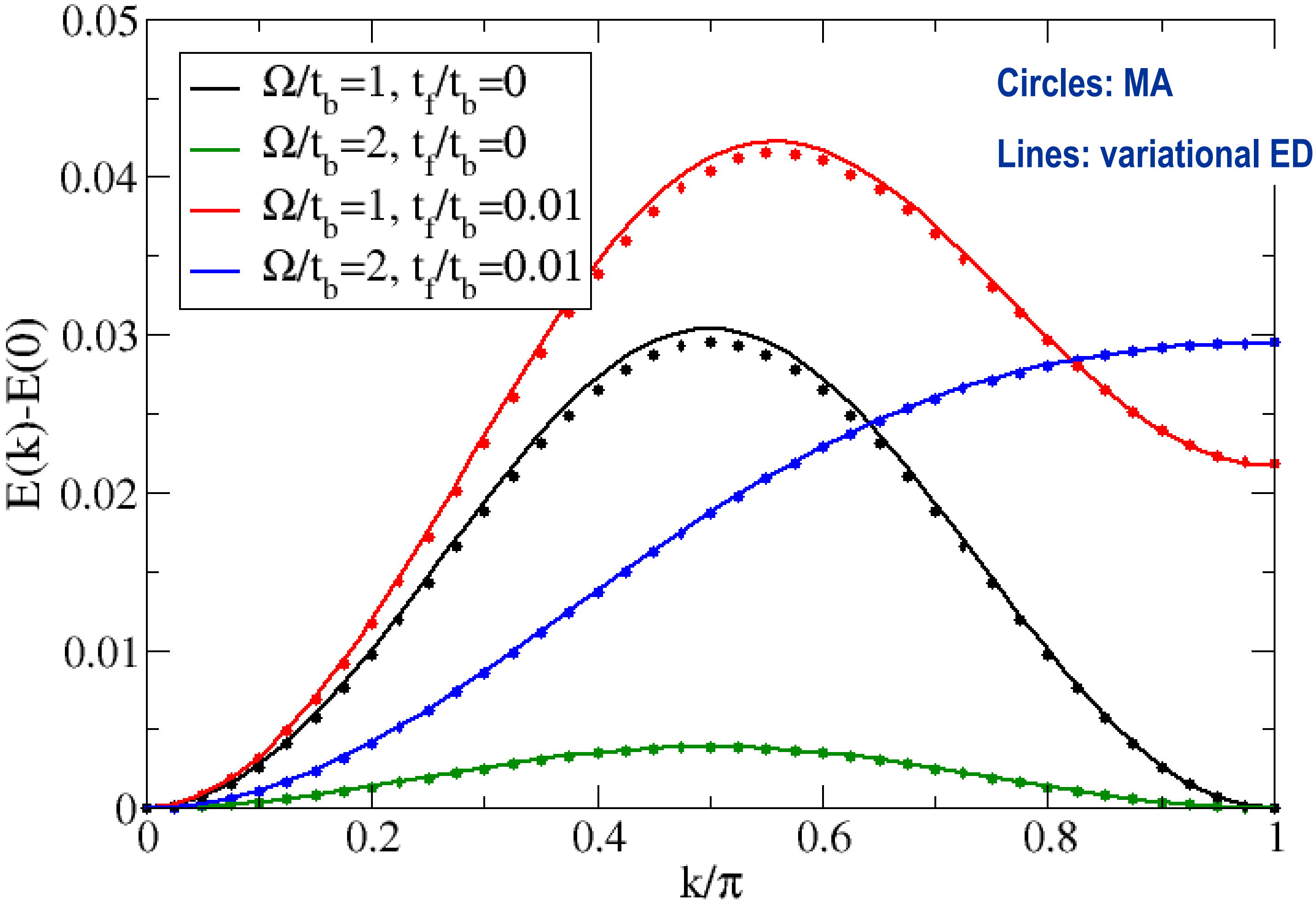
Note: even if t_f=0 can still dynamically generate a polaron mass through 3-boson, 3-site processes. The 1D version is not realistic for a spin background (cannot have hole at the same site as boson), but 2D is ok and it gives nnn hopping (Trugman loops).





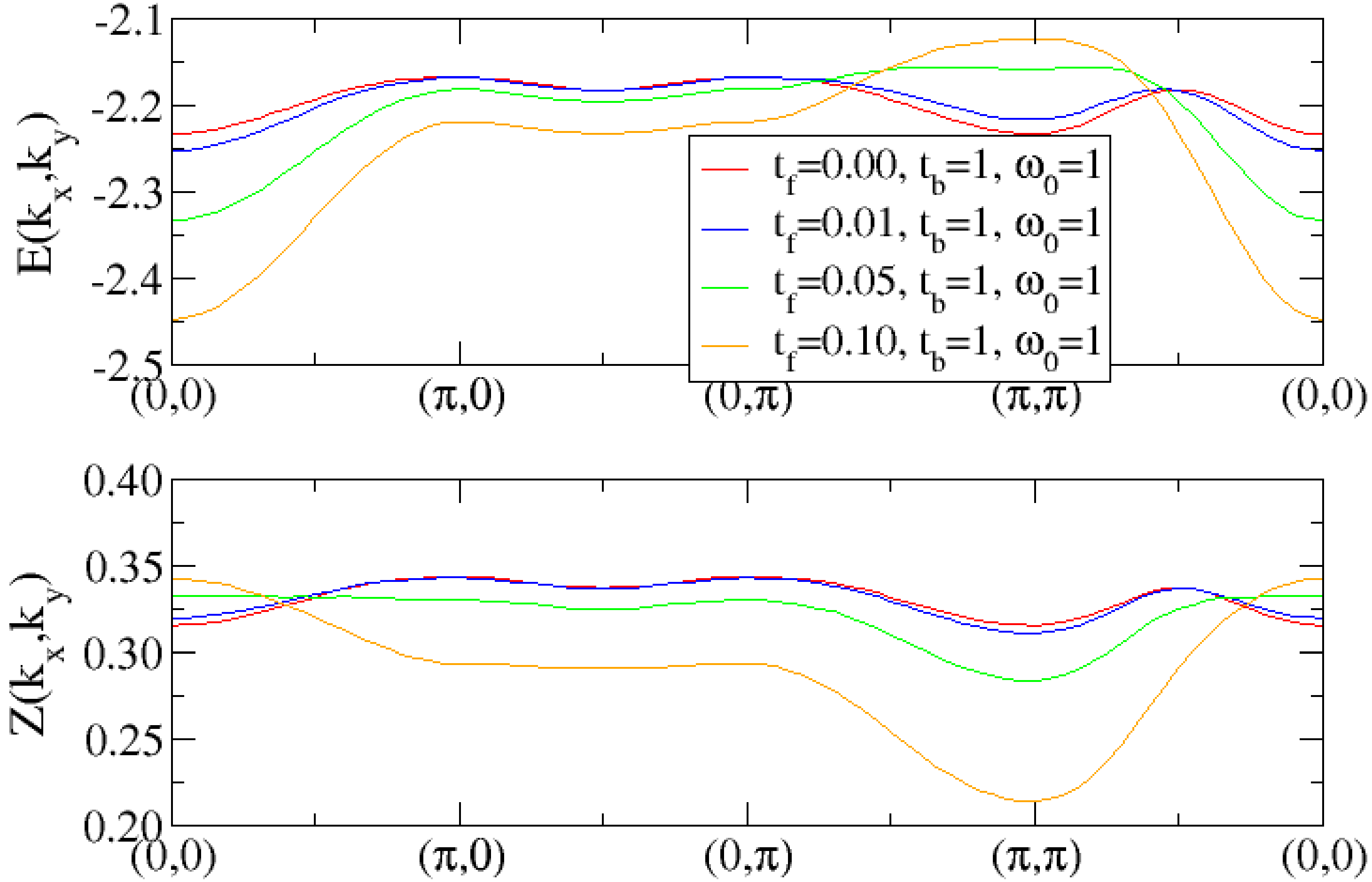
Such closed loops are ignored in the usual treatment of a hole in a tJ-model → usually SCBA = non-crossed diagrams only (bosons annihilated in inverse order to how they were created), whereas such loop processes correspond to maximally crossed diagrams (bosons annihilated in the same order they were created).

1D: good comparison with variational ED results. For t_f=0, indeed we see nnn hopping-like dispersion.



M. Berciu and H. Fehske, PRB 82, 085116 (2010)

2D: no available numerical results.



Indeed a large 2nd nn hopping arises and dominates dispersion at low t_f

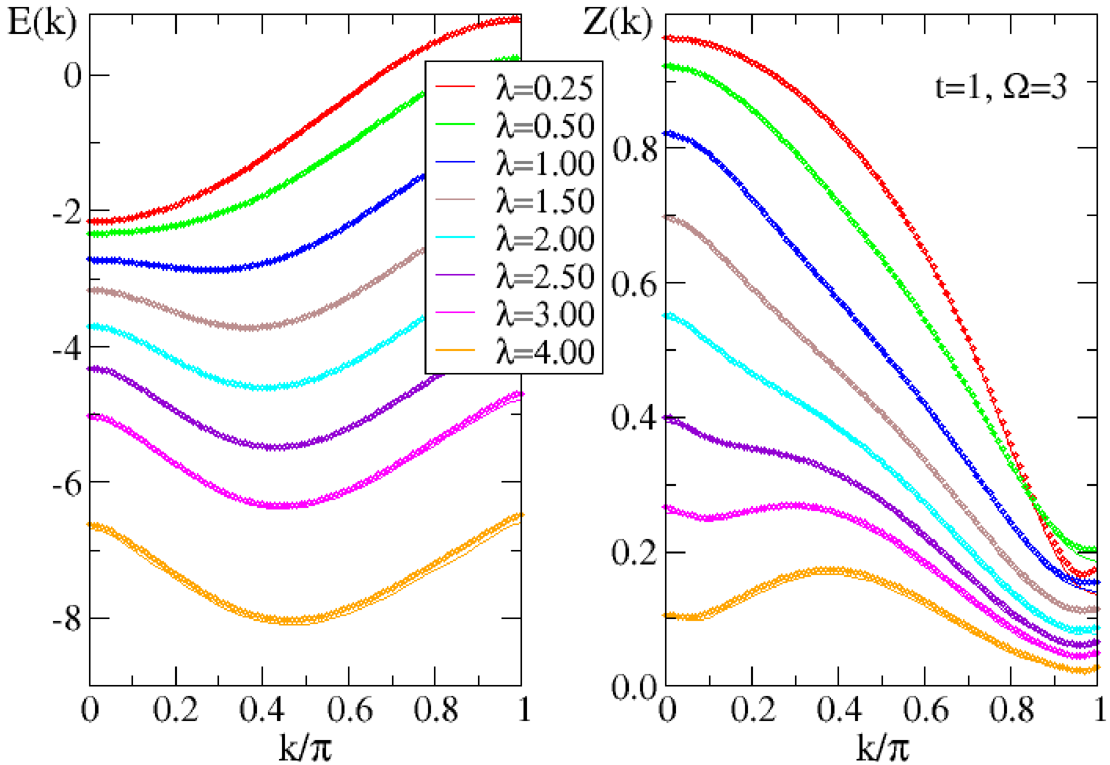
Model 2: phonon-modulated hopping like in polyacetylene (Su-Schrieffer-Heeger)

$$t_{i,i+1} \propto e^{-\alpha(R_{i+1}-R_i)} = t_0 e^{-\alpha(u_{i+1}-u_i)} \approx t_0[1-\alpha(u_{i+1}-u_i)]$$

$$u_i \propto b_i^\dagger + b_i$$

$$V_{\text{int}} = g\sum_i (c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1})[b_{i+1}^\dagger + b_{i+1} - b_i^\dagger - b_i]$$

→ as particle hops from one site to another, it can either create or annihilate a boson at either the initial or the final site.



Circles – MA

Lines - BDMC

Also very good agreement with data from G. de Filippis, V. Cataudella and A. Mishchenko and N. Nagaosa

PRL 105, 266605 (2010)

Momentum of GS switches from 0 (weak coupling) to finite value (strong coupling)

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

→ Such transitions impossible in models with g(q)

(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

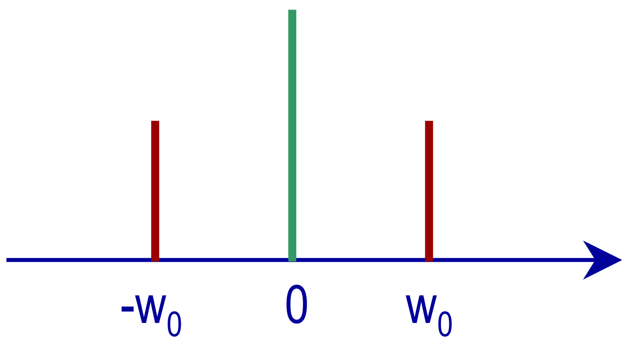
$$M_n(k) = \langle 0 | c_k H^n c_k^+ | 0 \rangle$$

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:



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

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

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

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

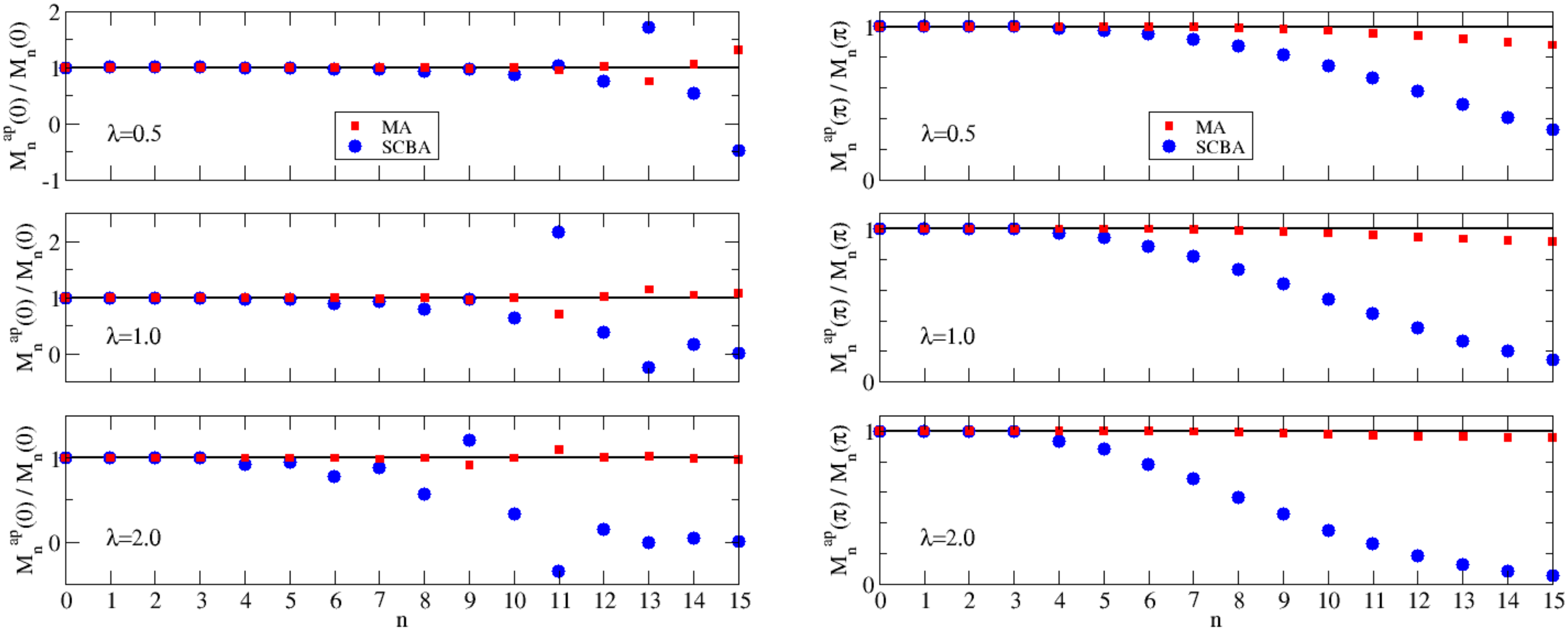
found correctly if n=0 diagram kept correctly → dominates if t >> g, λ → 0

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

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

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

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



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