Quasiparticles, dynamics, and coupled nanowires

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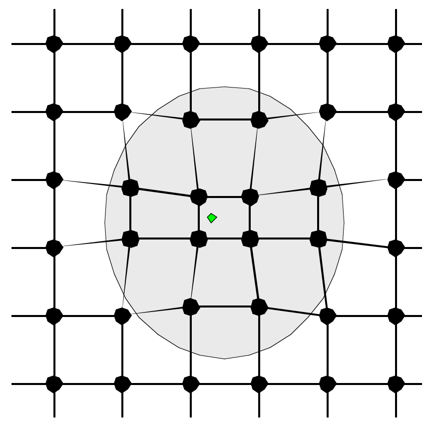
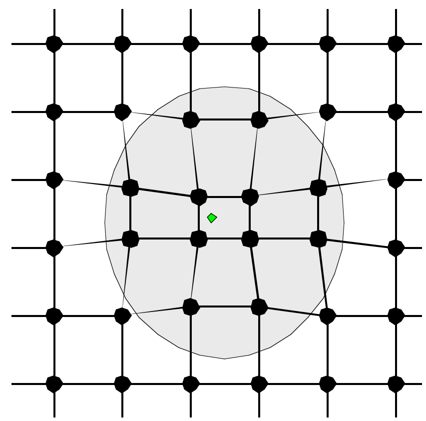
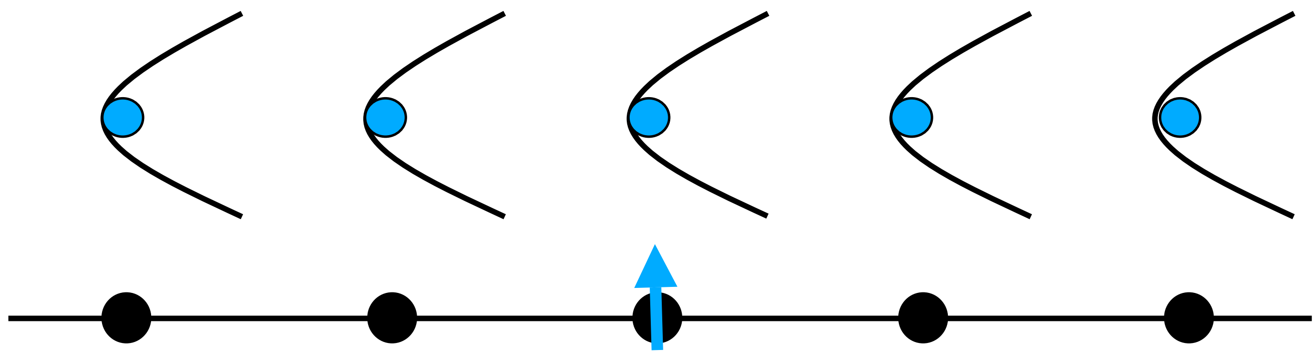
electron-phonon interaction

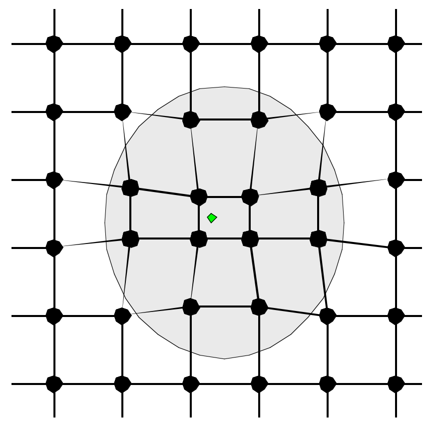


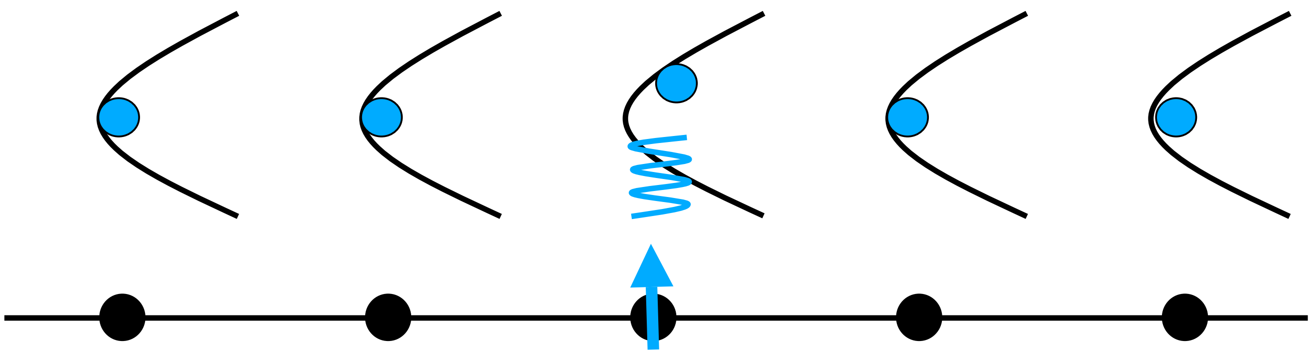
electron-phonon interaction





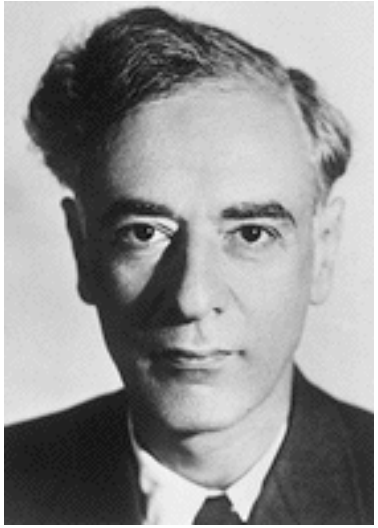
electron-phonon interaction

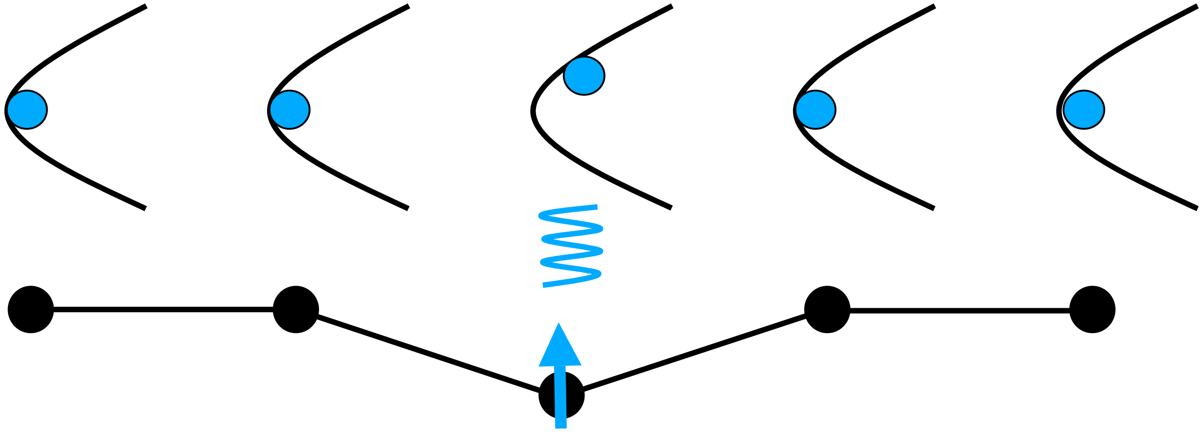




Lev Landau

L. D. Landau, Phys. Z. Sowjetunion 3, 644 (1933)





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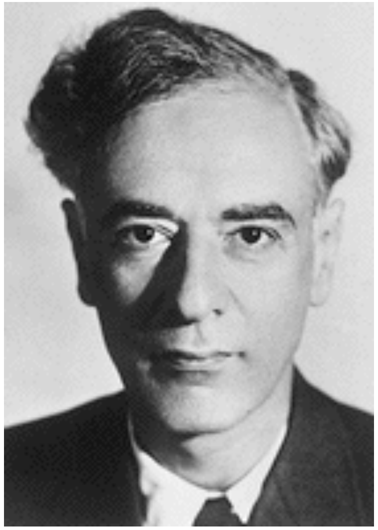
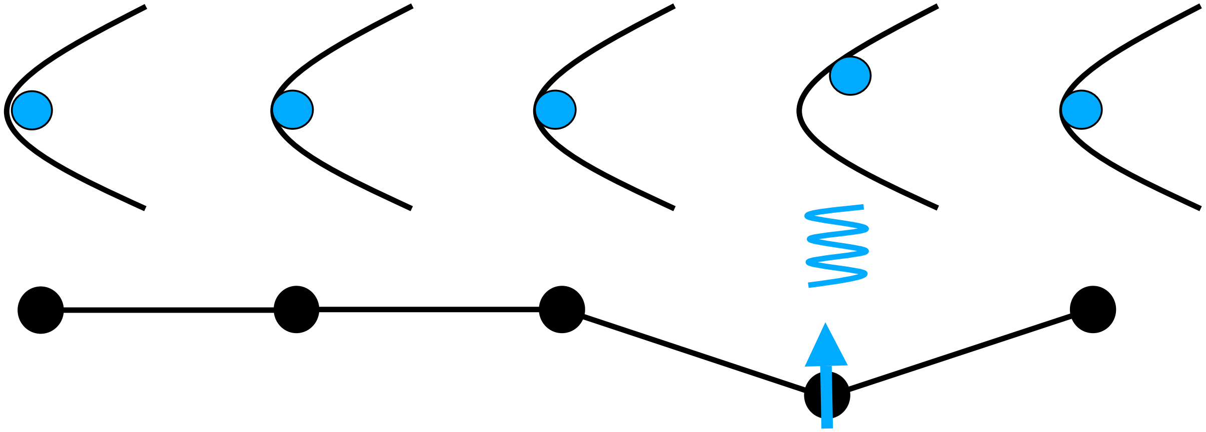
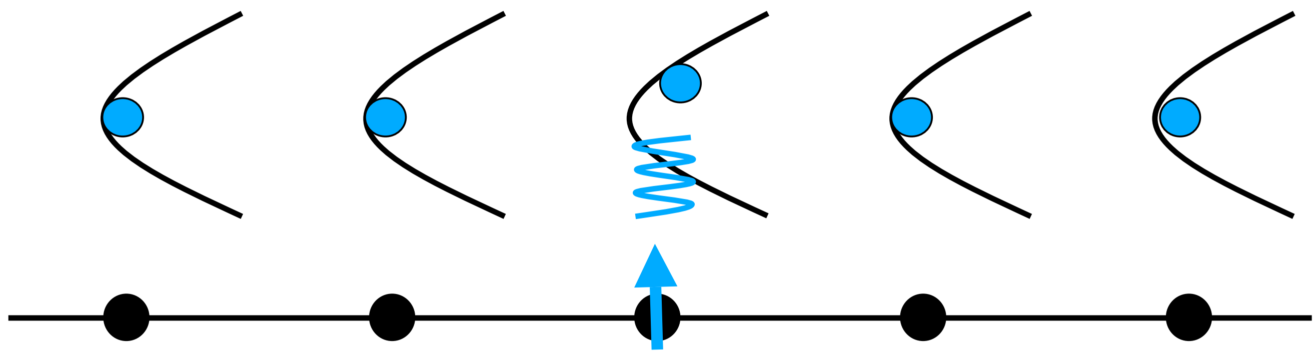




Holstein Hamiltonian

$$H = H_{el} + H_{ph} + H_{el-ph}$$
$$= -t \sum_{<i,j>} (c_i^\dagger c_j + h.c.) + \omega_0 \sum_i a_i^\dagger a_i - \lambda \sum_i c_i^\dagger c_i \underbrace{(a_i + a_i^\dagger)}_{x_i}$$



The two-site version of this problem maps exactly onto a spin-1/2 particle coupled to bosons.

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(but we will consider mainly the infinite lattice version in this talk)

It is common to make an approximation at this stage, such as the semiclassical approximation (classical phonons, quantum electrons),
or Born-Oppenheimer, surface hopping, ….
Problematic.

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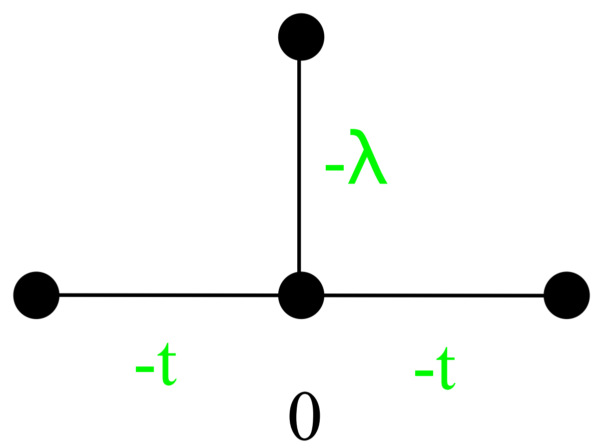
Problematic.

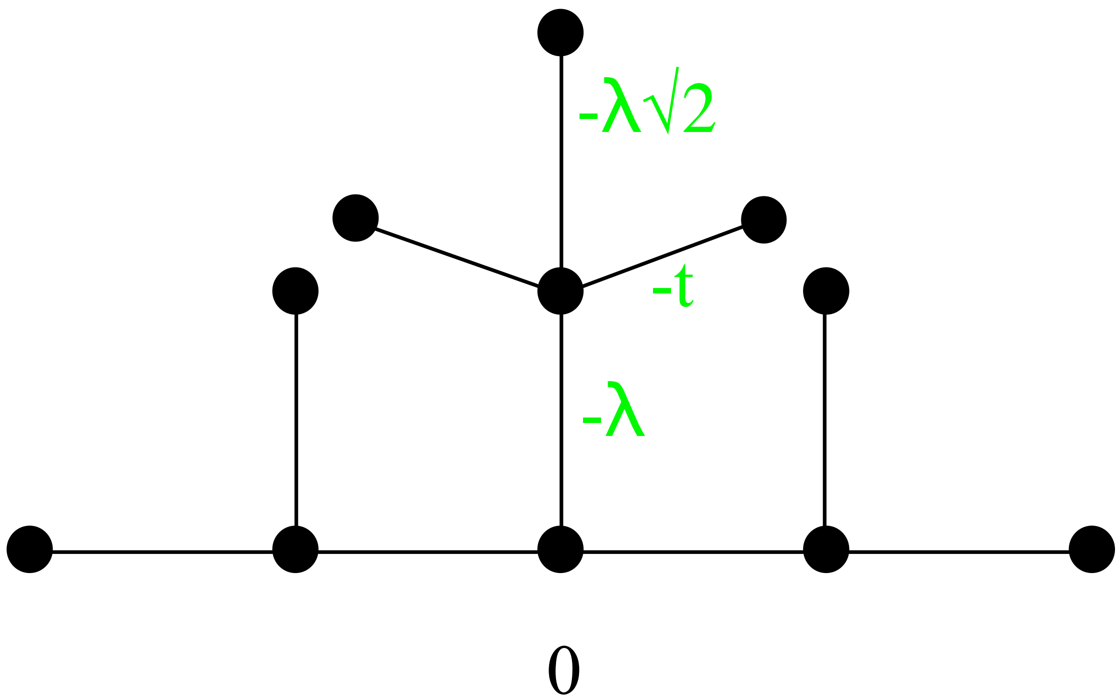
Numerically calculate quantum statics and dynamics in large variational many-body Hilbert space, including fully quantum phonons.
Numerically exact.

state space

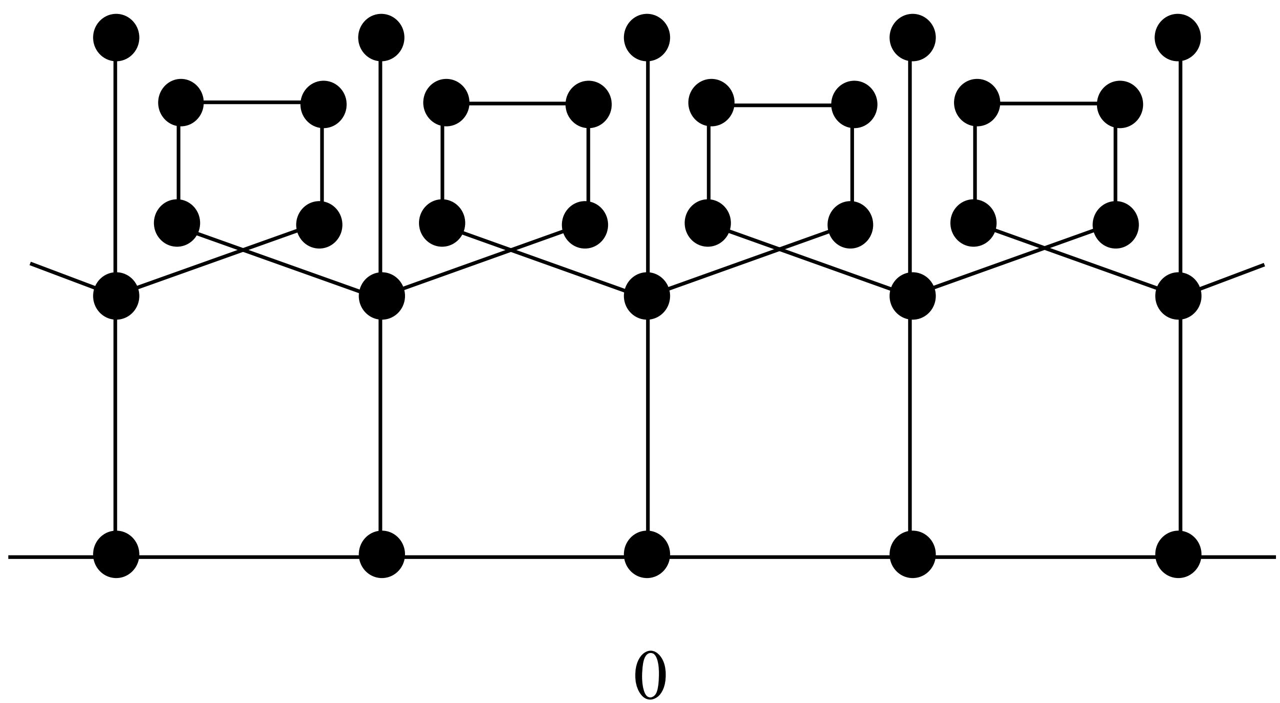
state space



state space



state space
(infinite lattice)



ground state energy $\lambda = \omega_0 = t = 1$

DMFT (dynamical mean-field)	-2.4	S. Cuichi *et.al*. Phys. Rev. B **56**, 4494 (1997)
Toyozawa	-2.456	Y. Toyozawa, Prog. Theor. Phys. **26**, 29 (1961)
Shore *et al.*	-2.464	H. B. Shore *et al*, Phys. Rev. B **7**, 4537 (1973)
QMC *(Monte-Carlo)*	-2.47	P. E. Kornilovitch, Phys. Rev. Lett. **81,** 5382 (1998)
Cataudella *et al.*	-2.467	V. Cataudella *et al.*, Phys. Rev. B **62**, 1496 (2000)
GL variational method	-2.4693	A. H. Romero *et al.*, J Chem. Phys. **109**, 6540 (1998)
DMRG	-2.46968	E. Jeckelman *et al.*, Phys. Rev. B **57**, 6376 (1998)
Finite-Cluster ED	-2.4696847	W. Wellein *et al.*, Phys. Rev. B **56**, 4513 (1997)
VED	-2.469684723932870715 61	Li-Chung Ku *et al.*, Phys. Rev. B. **65**, 174306 (2002), …

Dynamics of quasiparticle formation in electron-phonon coupled systems.

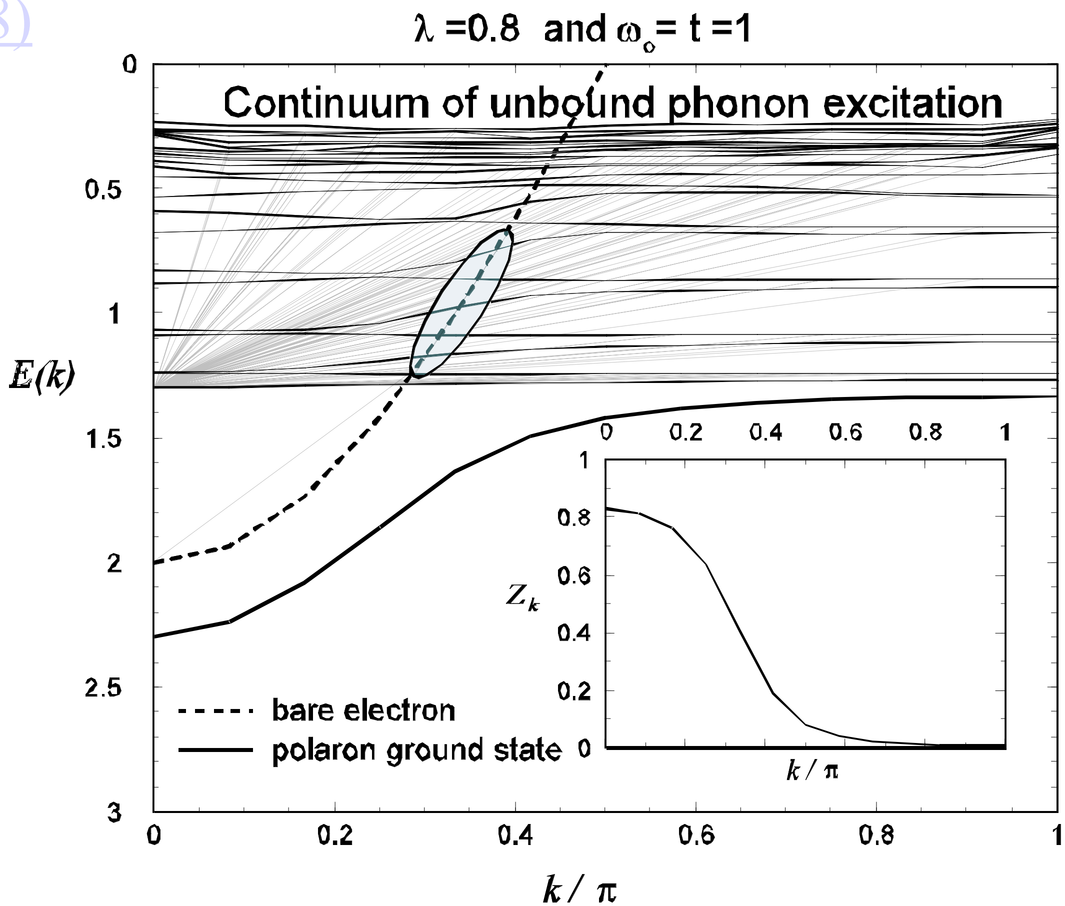
- How are phonons excited and how do they evolve into the correlated phonon cloud of the polaron quasiparticle?
- How much time does it take to form a polaron from a bare (delocalized) electron?
- What is the effect of dimension on the dynamics of polaron formation?

$$i\frac{d\psi}{dt} = H\psi$$

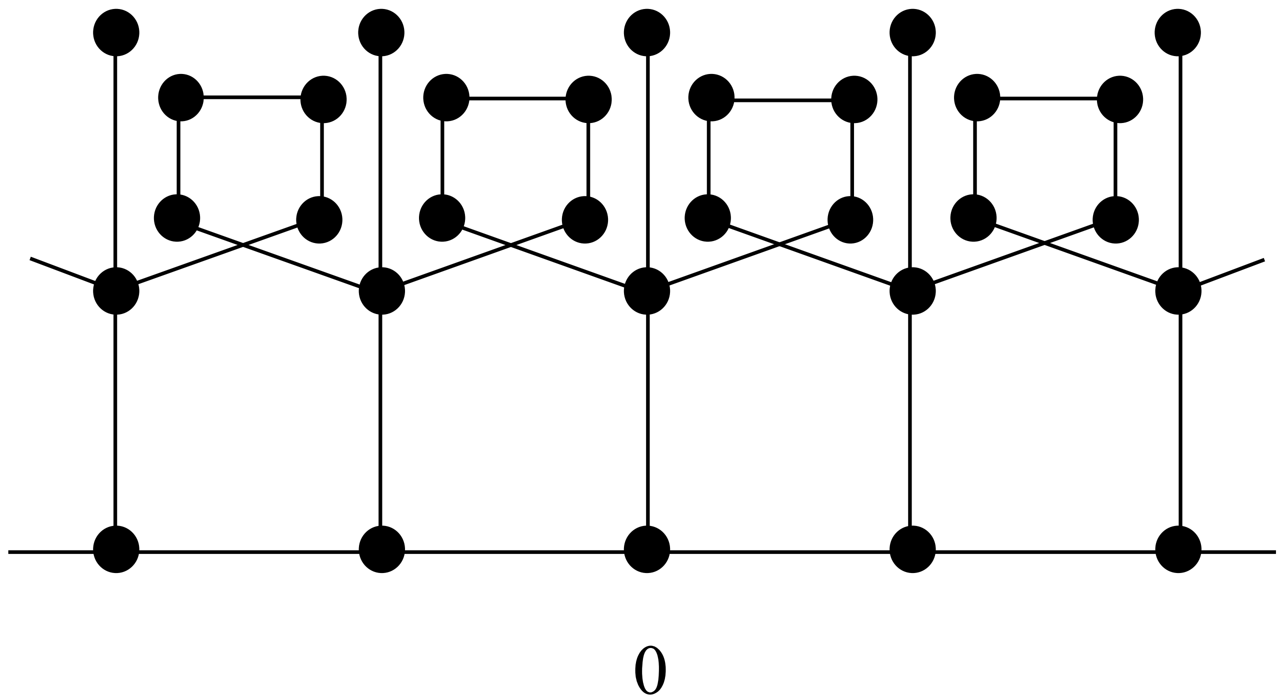
Quantum Dynamics

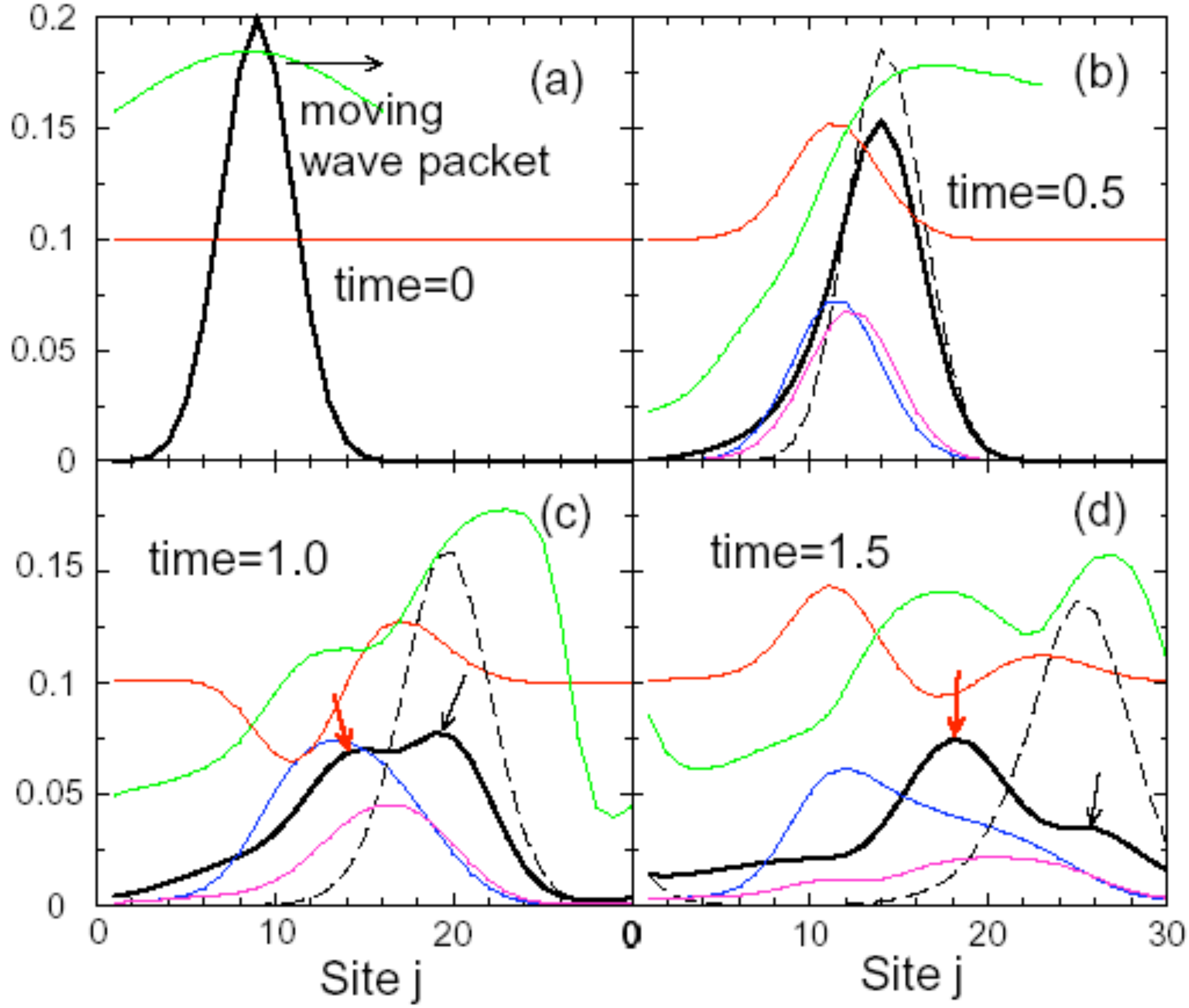
- Movie I (lambda=0.4)
- Movie II (lambda=0.8)

Polaron Energy Dispersion



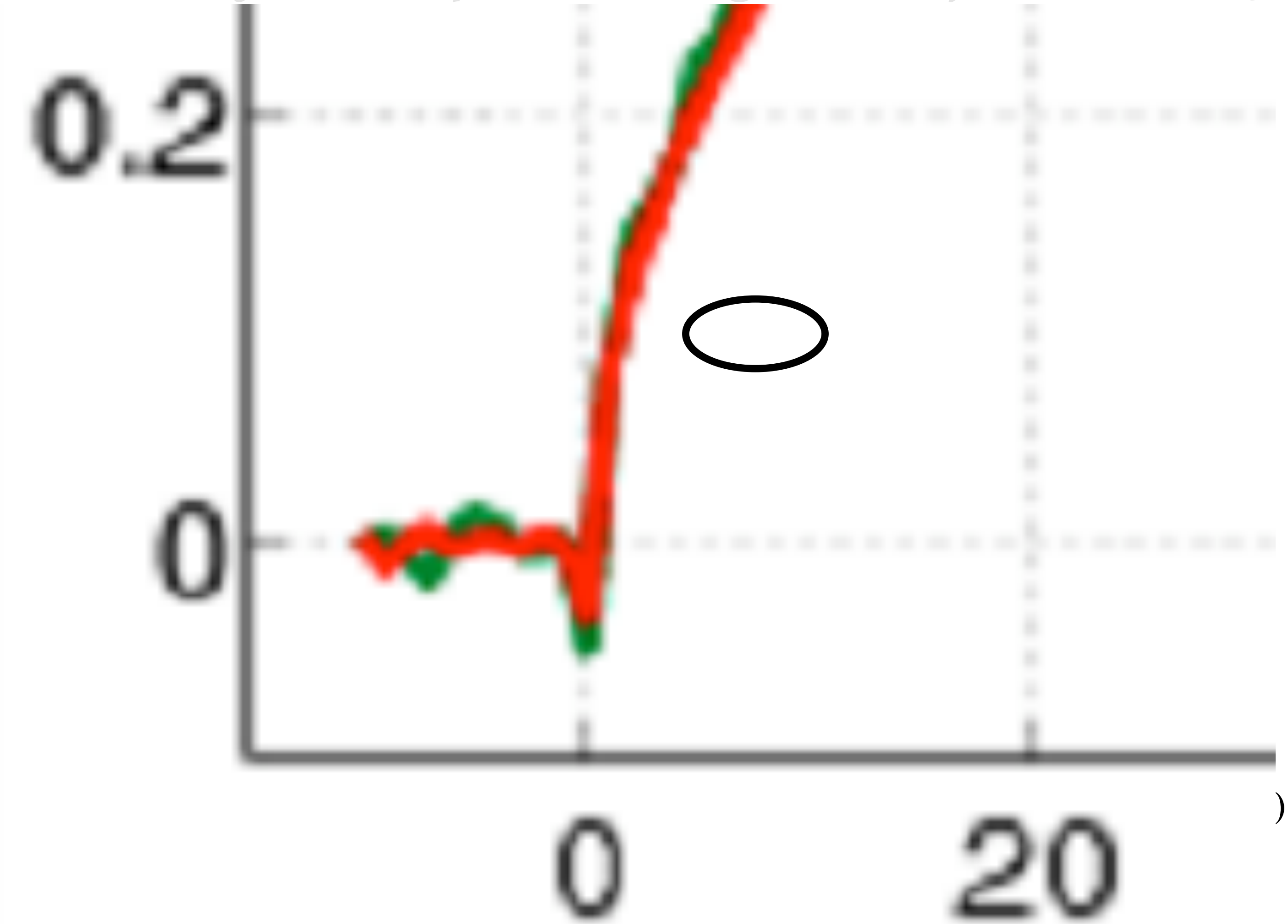
state space
(infinite lattice)





0.2
0.15
0.1
0.05
0
(a)
moving
wave packet
time=0
(b)
time=0.5
(c)
time=1.0
(d)
time=1.5
0
10
20
0
10
20
30
Site j
Site j

LCMO: Comparison of all-optical (ΔA / A) and THz (Δσ) data reveals dynamic spectral weight transfer: below T_c



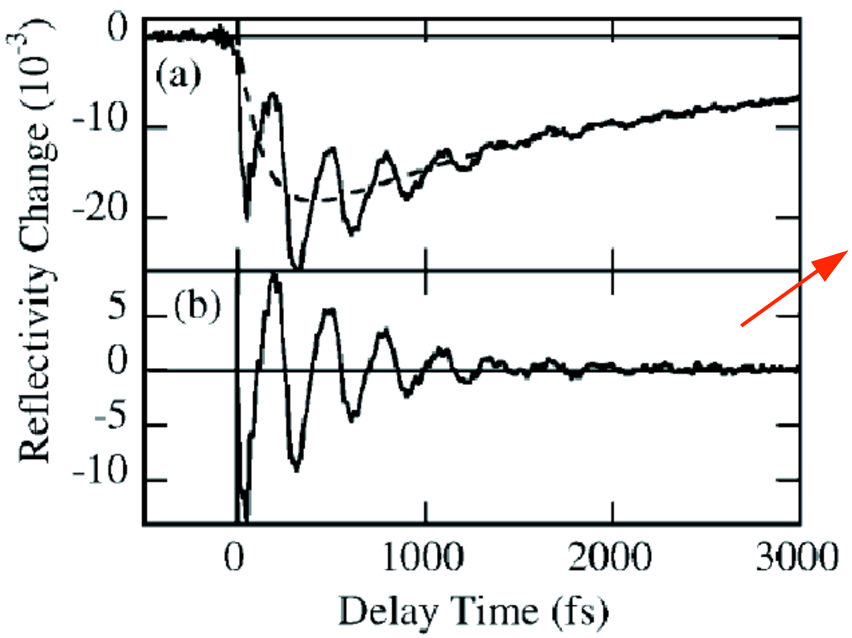
).

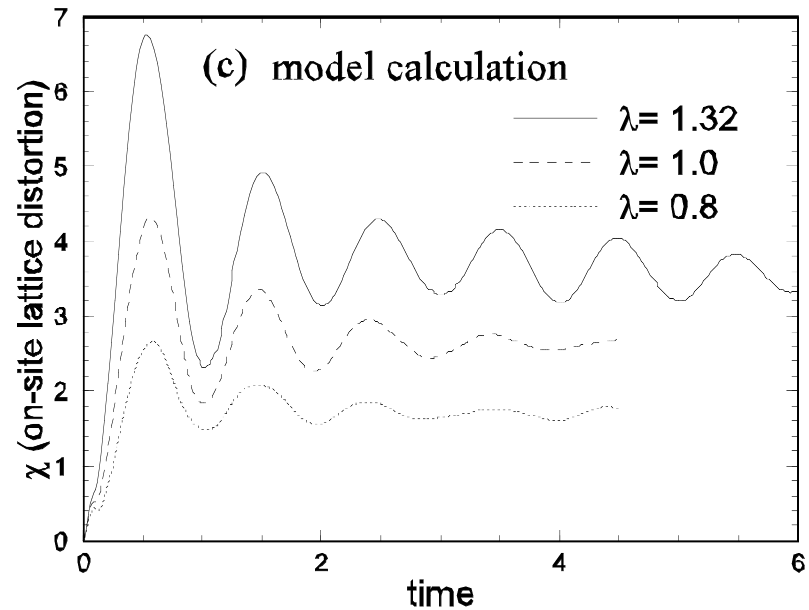
A. J. Taylor et al.

Time (ps)

Optical pump-probe on MX chain, PtI, quasi-1D, excitons

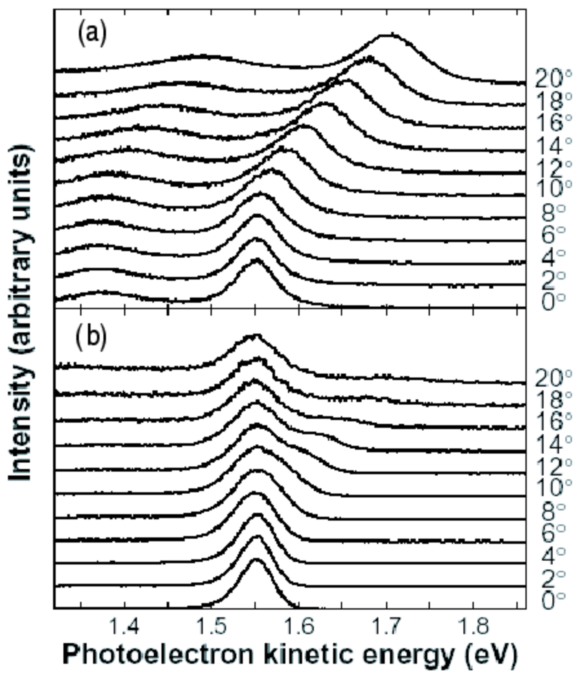
This work



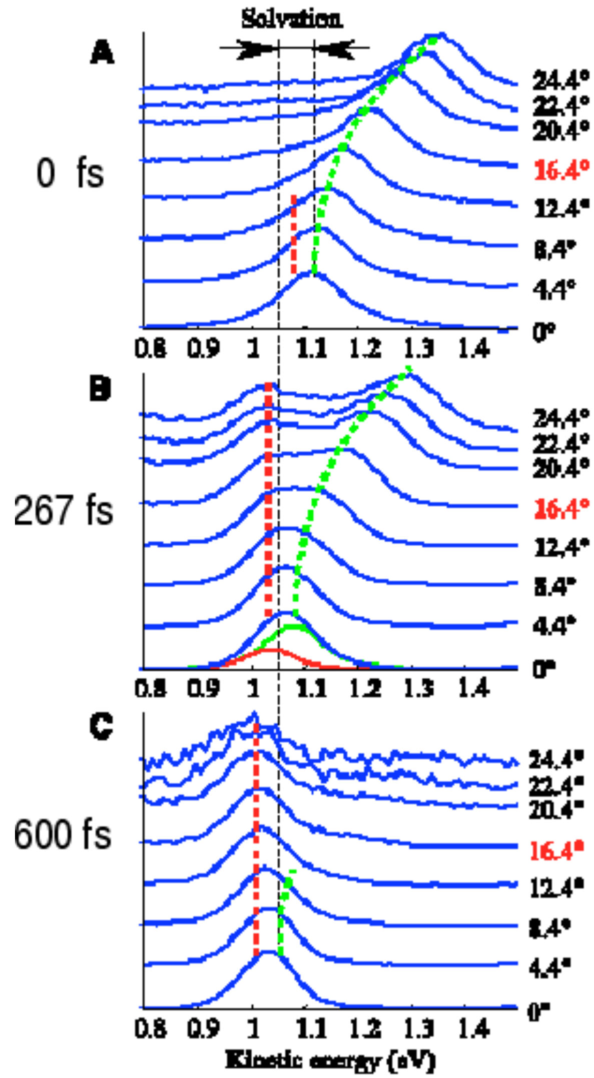


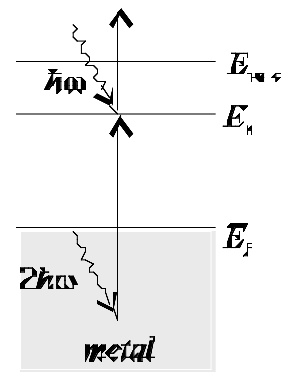
A. Sugita et al., PRL **86**, 2185 (2001)

Two-photon photoemission, alkanes on Ag, Harris et al.



N.-H Ge et al, Science **279**, 202 (1998)



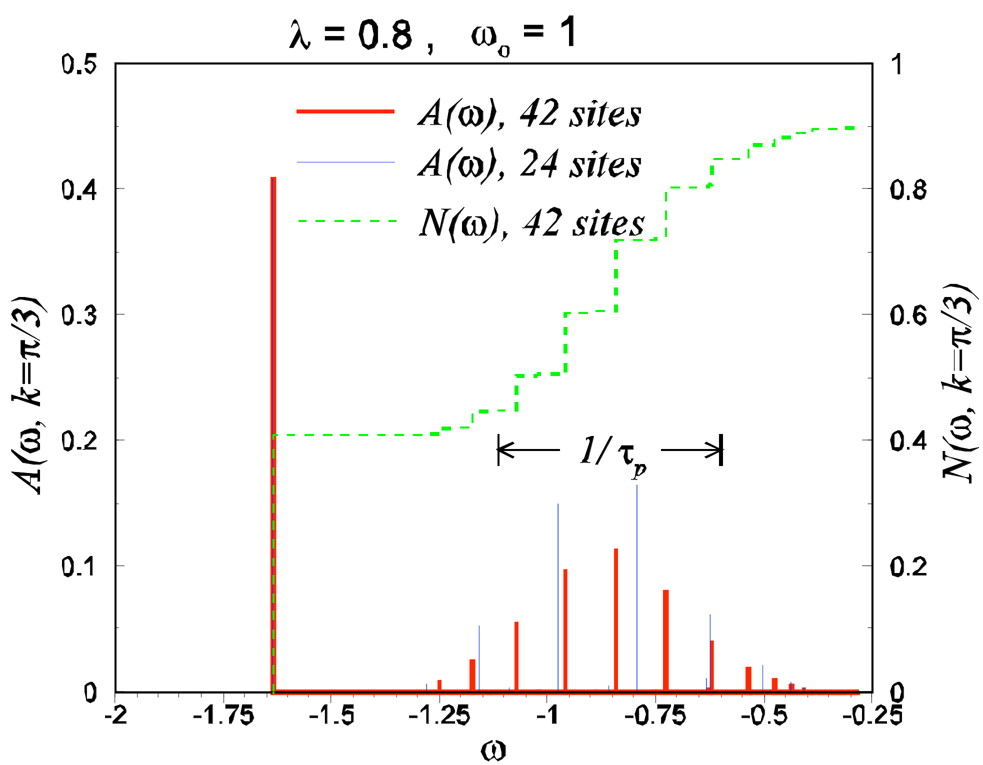


A.D. Miller et al, Science **297**, 1163 (2002)

$$
\begin{aligned}
|\psi(t>0)\rangle &= \sum_{n=0}^{\infty} e^{-iE_n t}|\Psi_n\rangle\langle\Psi_n|\psi(0)\rangle \\
&= e^{-iE_0 t}|K_{pol}\rangle\langle K_{pol}|\psi(0)\rangle + \sum_{q1} e^{-iE_{q_1} t}|K_{pol},\ q_1\rangle\langle K_{pol},\ q_1|\psi(0)\rangle \\
&+ \sum_{q_1,q_2} e^{-iE_{q_1,q_2} t}|K_{pol},\ q_1,q_2\rangle\langle K_{pol},\ q_1,q_2|\psi(0)\rangle \ + \ \ldots \\
&= \text{quasiparticle amplitude} + \text{unbound phonon excitation}
\end{aligned}
$$

Spectral Function

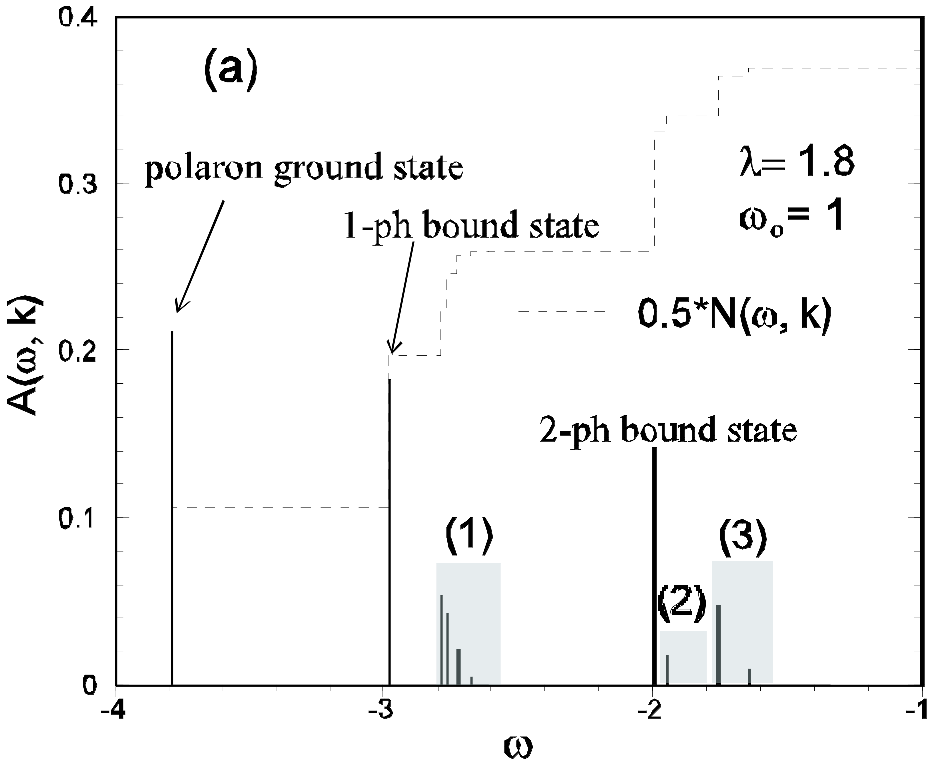
$$A(\omega,k) = \sum_n \left|\langle \Psi_n | c_k^\dagger | 0 \rangle\right|^2 \delta(\omega - E_n)$$



Quasiparticle excited states

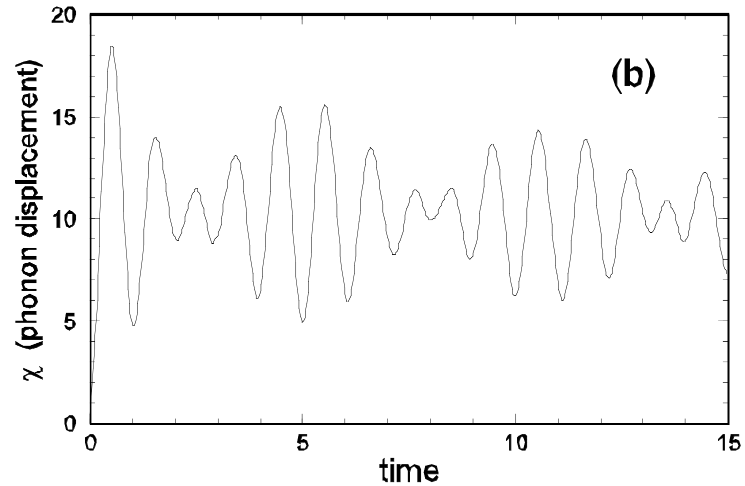
(*strong coupling*)

Spectral function



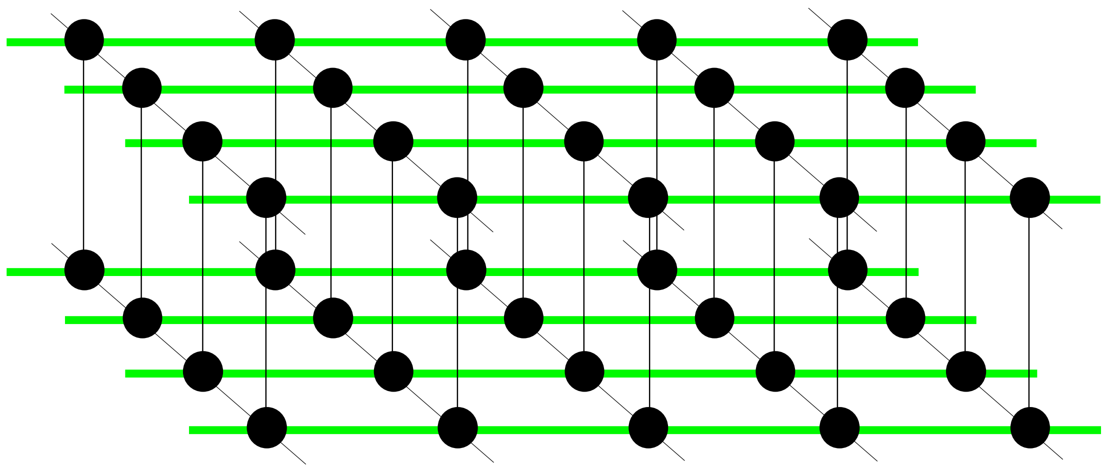
On-site lattice distortion

$$\chi = \left\langle c_0^\dagger c_0 \left(a_0 + a_0^\dagger\right)\right\rangle$$



Quantum beat

Coupled quantum wires
From 1d to 3d



Previous work, classical approximation,
infinite mass phonons,
1d qualitatively different than 3d (Emin).

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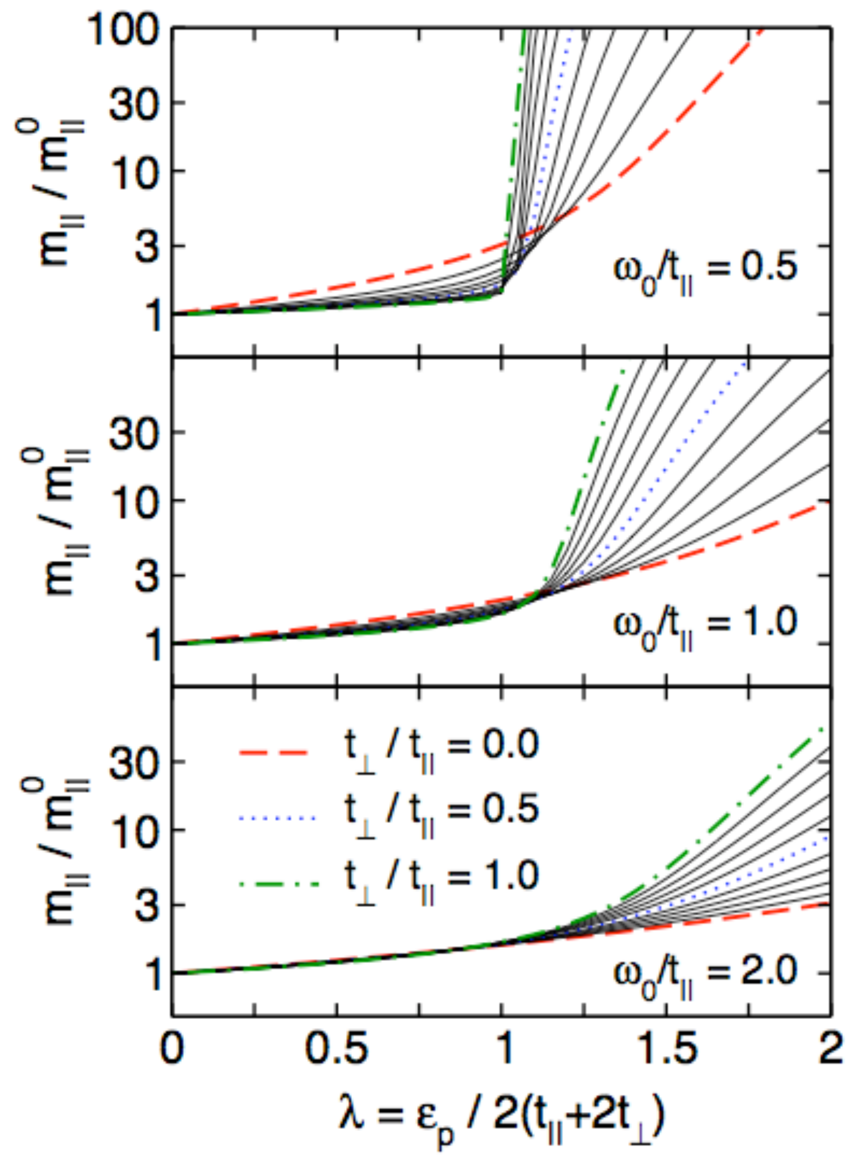
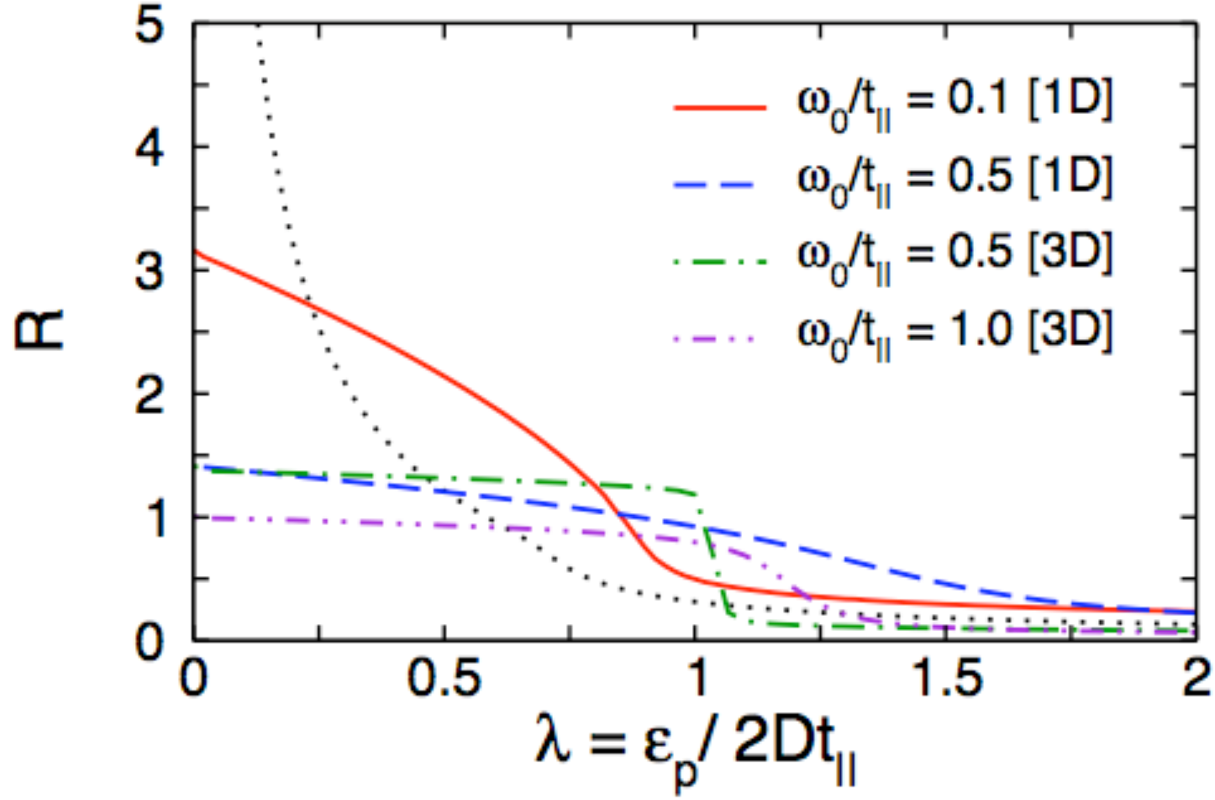
infinite mass phonons,
1d qualitatively different than 3d (Emin).

What happens when you continuously connect
two limits that cannot be connected?



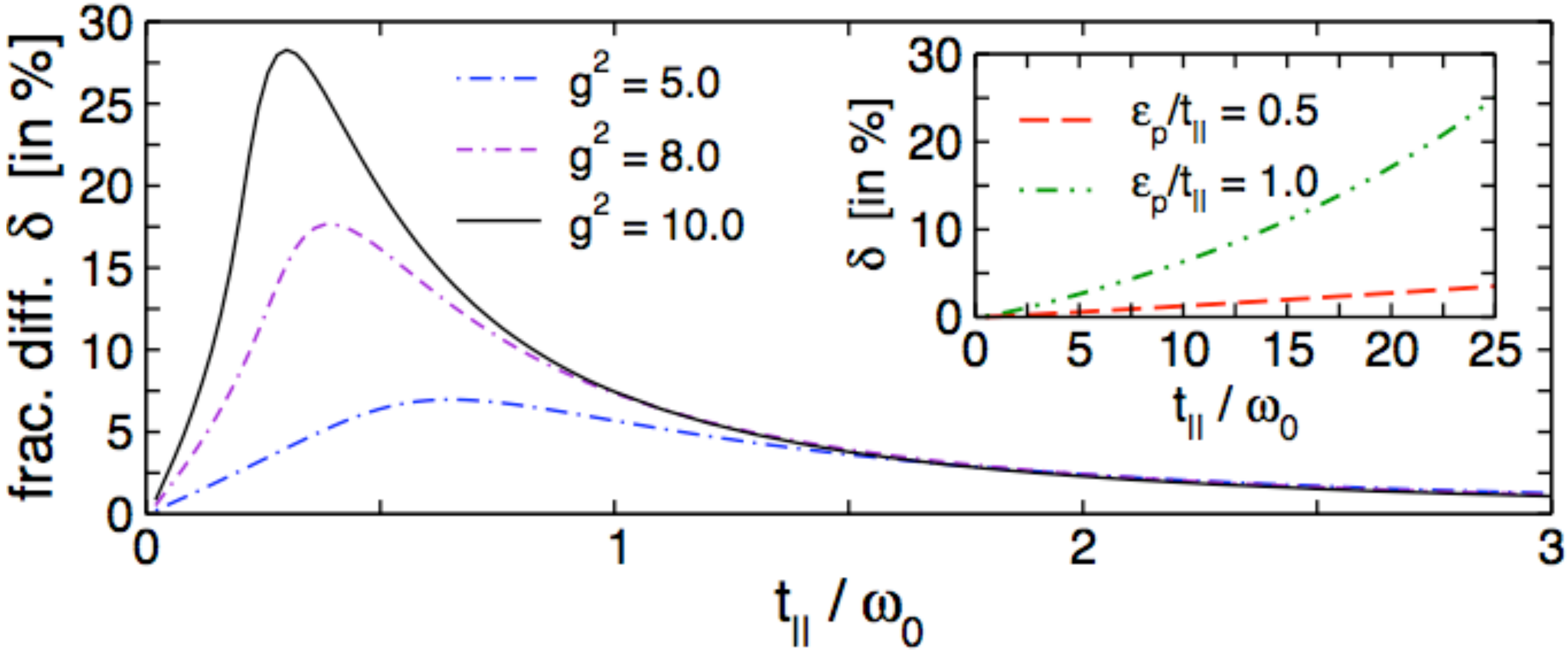
Quasiparticle effective mass as a function of el-ph coupling (fully quantum)



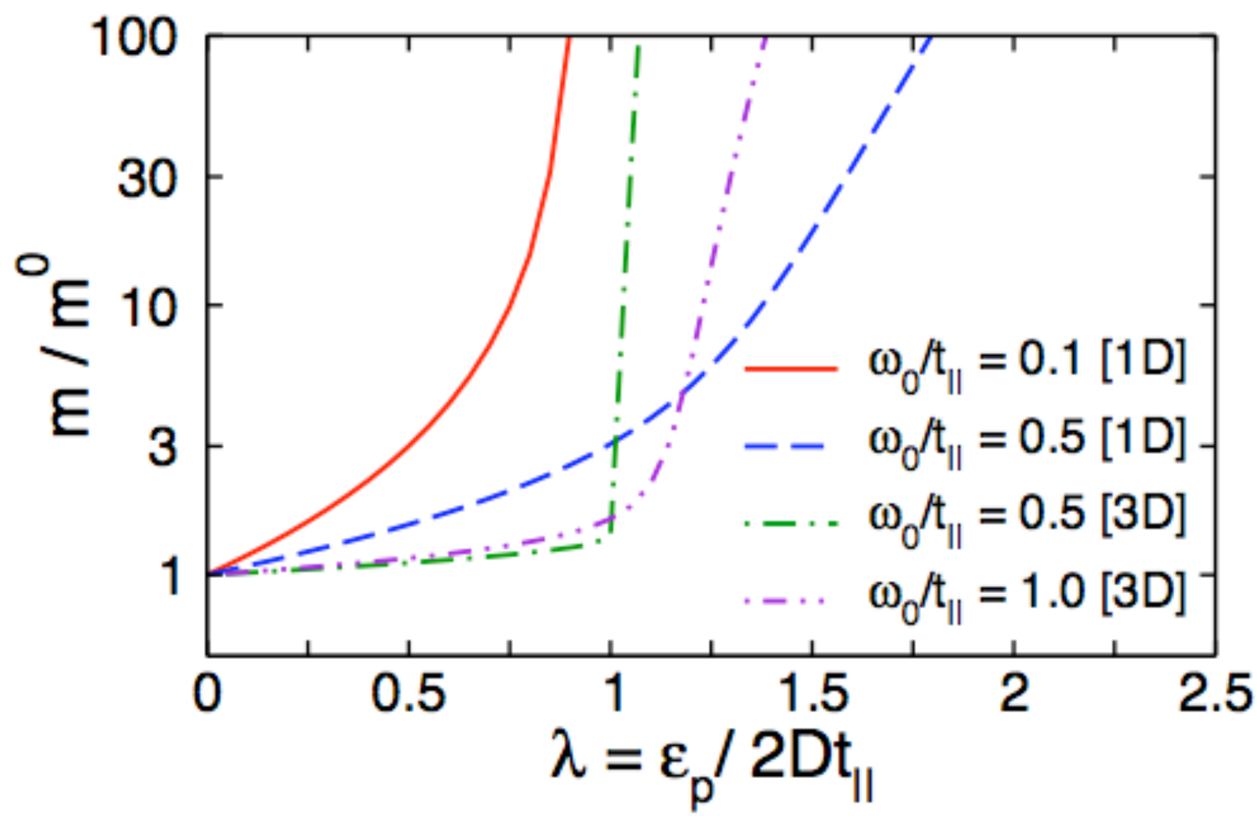
Polaron radius as a function of el-ph coupling.

Increasing the el-ph coupling causes the mass to increase in both the parallel and perpendicular directions.

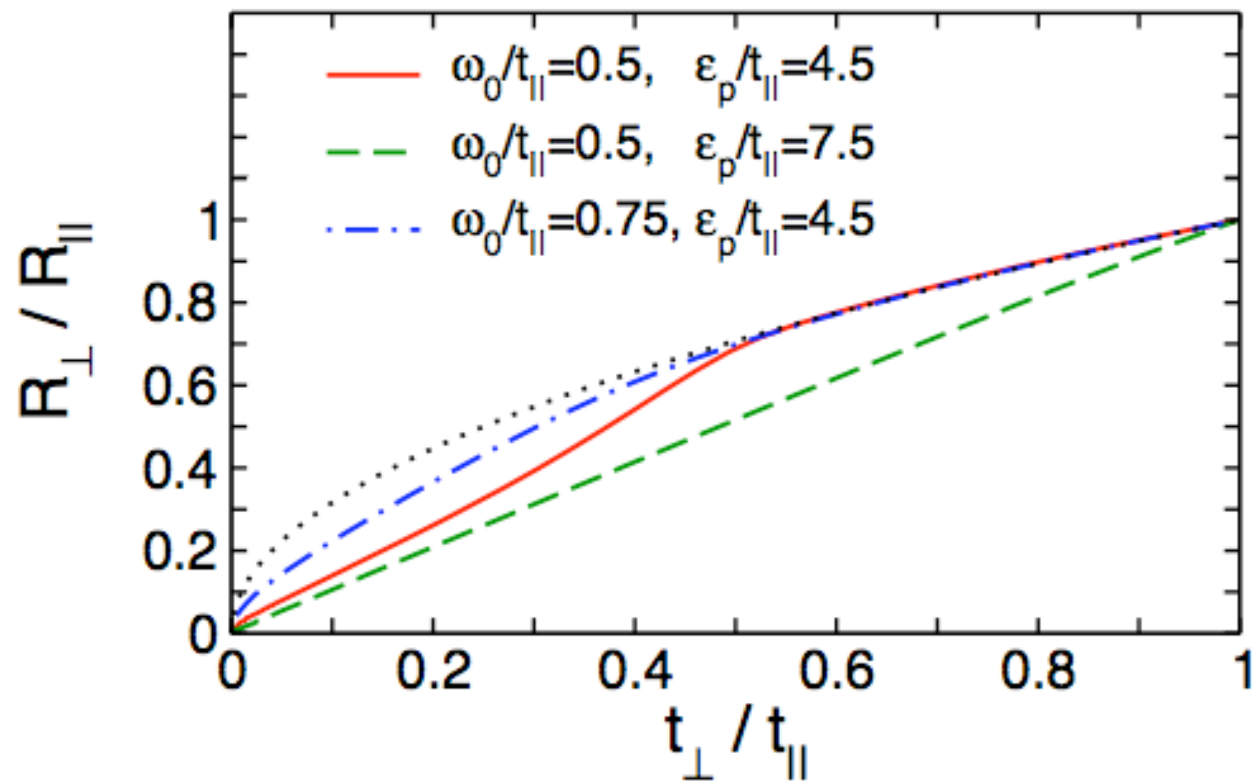
By the same amount?



Additional mass enhancement in the perpendicular direction compared to the parallel direction.



100
30
10
3
1
m / m^0
0
0.5
1
1.5
2
2.5
λ = ε_p / 2Dt_||
ω_0/t_|| = 0.1 [1D]
ω_0/t_|| = 0.5 [1D]
ω_0/t_|| = 0.5 [3D]
ω_0/t_|| = 1.0 [3D]



ω0/t|| =0.5, εp/t|| =4.5
ω0/t|| =0.5, εp/t|| =7.5
ω0/t|| =0.75, εp/t|| =4.5
R⊥ / R||
t⊥ / t||
0
0.2
0.4
0.6
0.8
1

collaborators

Li-Chung Ku
Janez Bonca
Holger Fehske
Andreas Alvermann

Richard Averitt
Rohit Prasankumar
Antoinette Taylor
Sue Dexheimer

Summary

1. The properties of quasiparticles are of general interest (condensed matter, high energy). This approach is applicable to other kinds of quasiparticles, such as the spin polaron (htc) and the exciton dressed by phonons.
2. Calculated the fully quantum ground state, excited states, and dynamics far from equilibrium of quasiparticle formation in real time and real space in a large many-body Hilbert space.
3. Calculated the properties of coupled quantum wires, 1d to 3d crossover.

References:

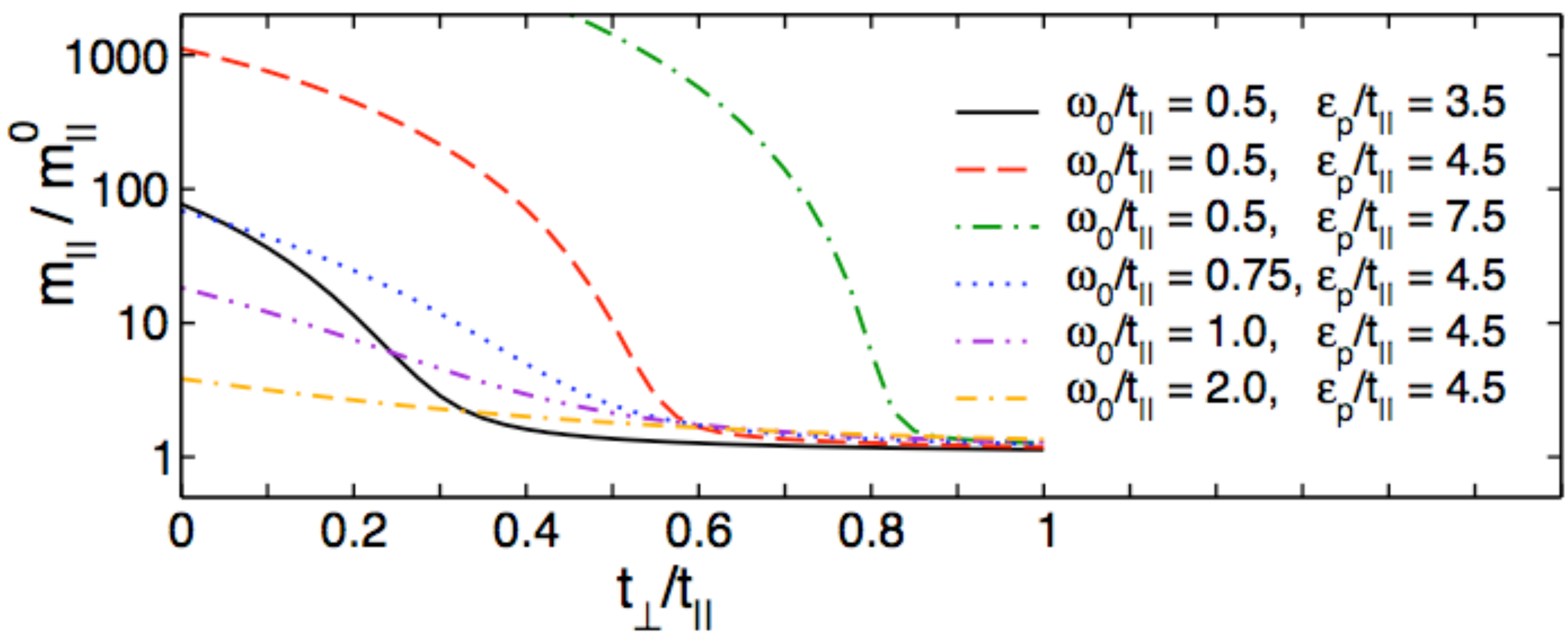
unpublished; and

Alvermann, Fehske, ST, PRB 78, 165106 (2008).

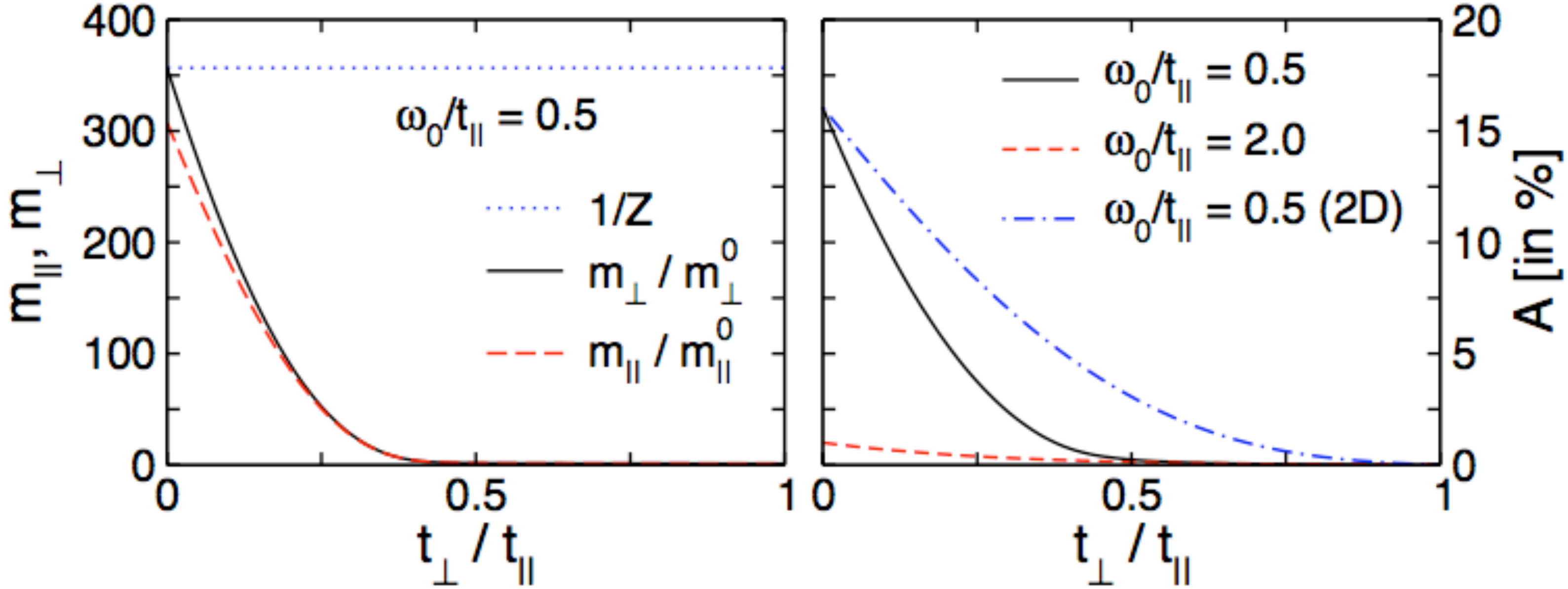
Ku, ST, PRB 75, 014307 (2007).

Demsar, Averitt, Ahn, Graf, ST, Kabanov, Sarrao, Taylor, PRL 91, 027401 (2003).

Ku, ST, Bonca, PRB 65, 174306 (2002).

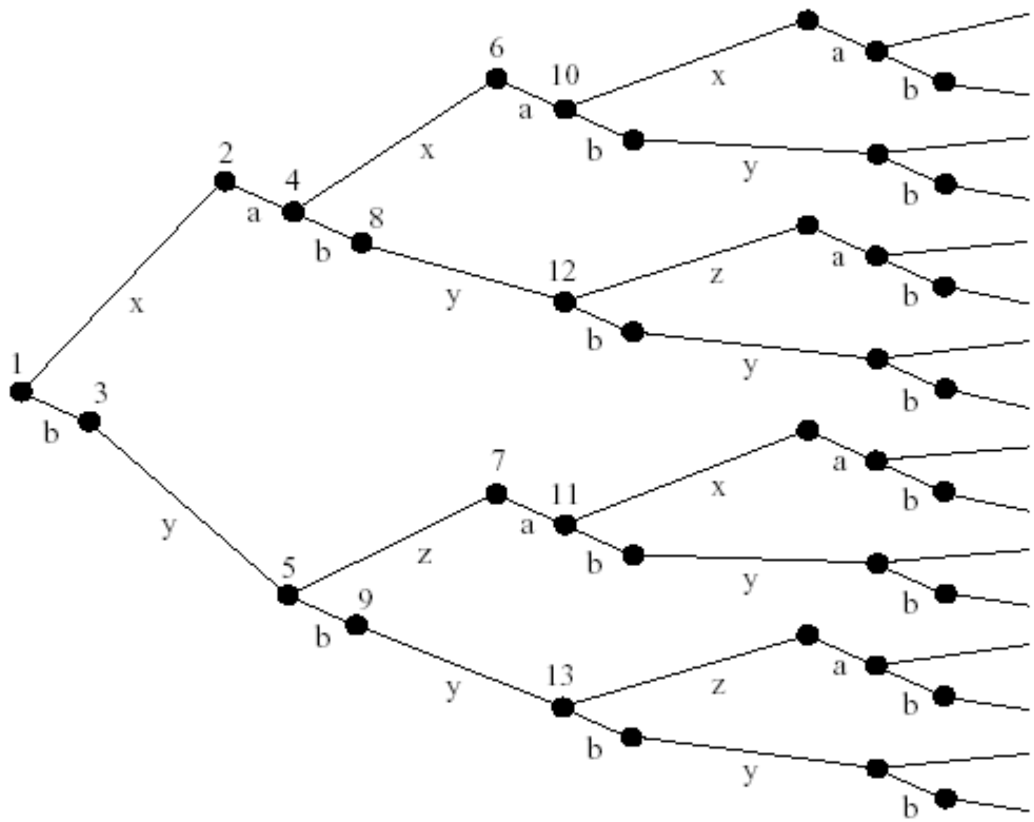


1000
100
10
1
0
0.2
0.4
0.6
0.8
1
$m_{||} / m_{||}^0$
$t_\perp / t_{||}$
$\omega_0/t_{||}$ = 0.5, $\varepsilon_p/t_{||}$ = 3.5
$\omega_0/t_{||}$ = 0.5, $\varepsilon_p/t_{||}$ = 4.5
$\omega_0/t_{||}$ = 0.5, $\varepsilon_p/t_{||}$ = 7.5
$\omega_0/t_{||}$ = 0.75, $\varepsilon_p/t_{||}$ = 4.5
$\omega_0/t_{||}$ = 1.0, $\varepsilon_p/t_{||}$ = 4.5
$\omega_0/t_{||}$ = 2.0, $\varepsilon_p/t_{||}$ = 4.5

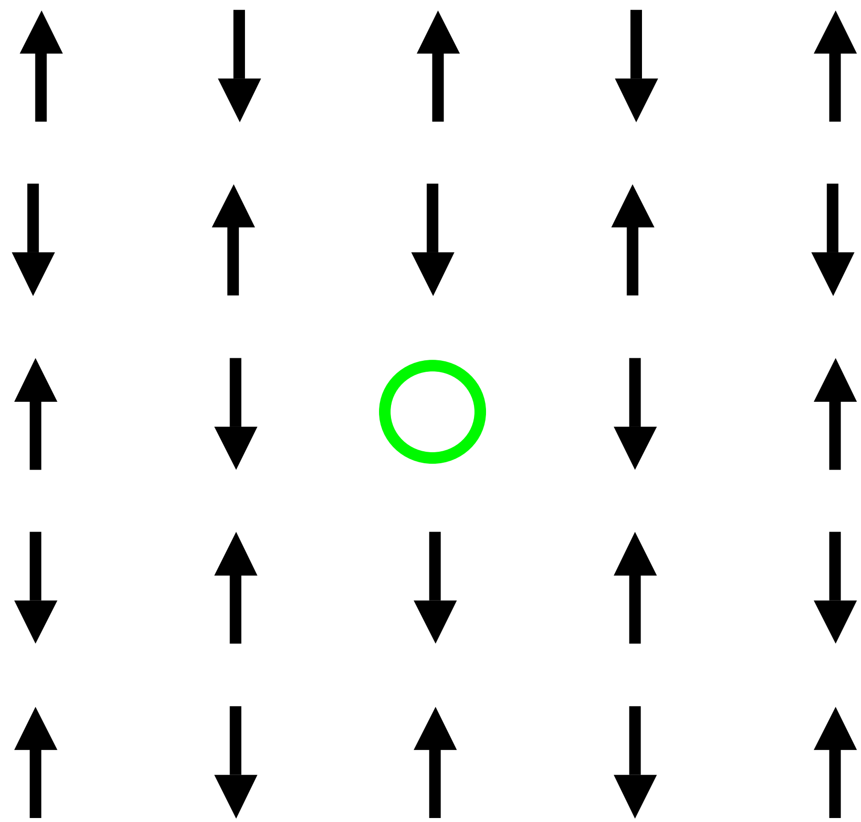


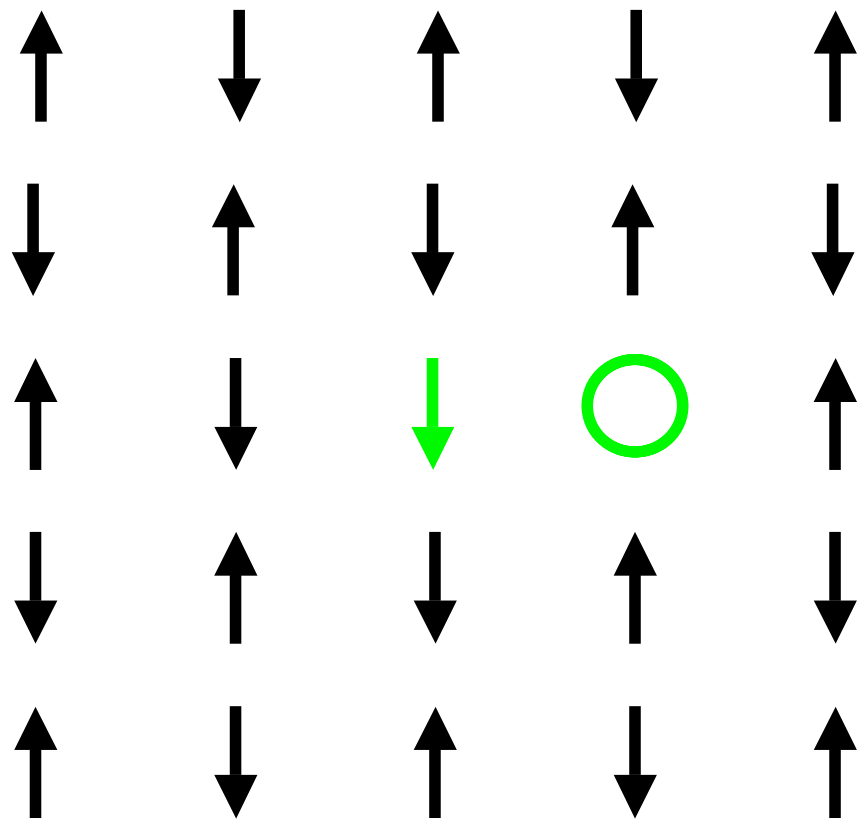
400
300
200
100
0
$m_{||}$, $m_\perp$
$\omega_0/t_{||}$ = 0.5
1/Z
$m_\perp$ / $m_\perp^0$
$m_{||}$ / $m_{||}^0$
0
0.5
1
$t_\perp$ / $t_{||}$
$\omega_0/t_{||}$ = 0.5
$\omega_0/t_{||}$ = 2.0
$\omega_0/t_{||}$ = 0.5 (2D)
20
15
10
5
0
A [in %]
0
0.5
1
$t_\perp$ / $t_{||}$

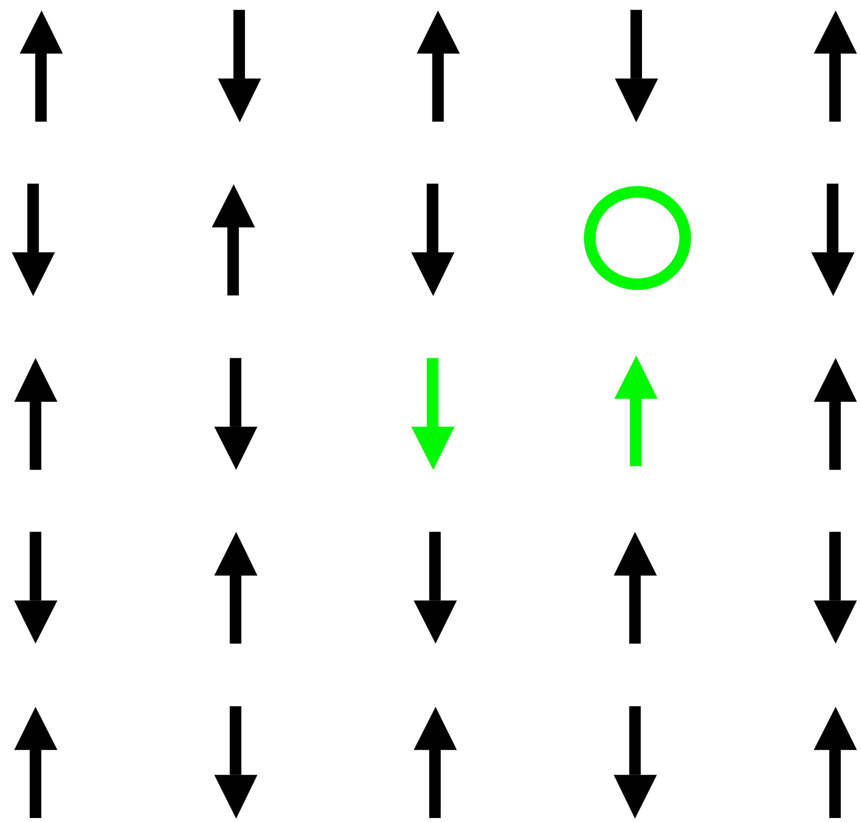
state space
electron and phonons in electric field



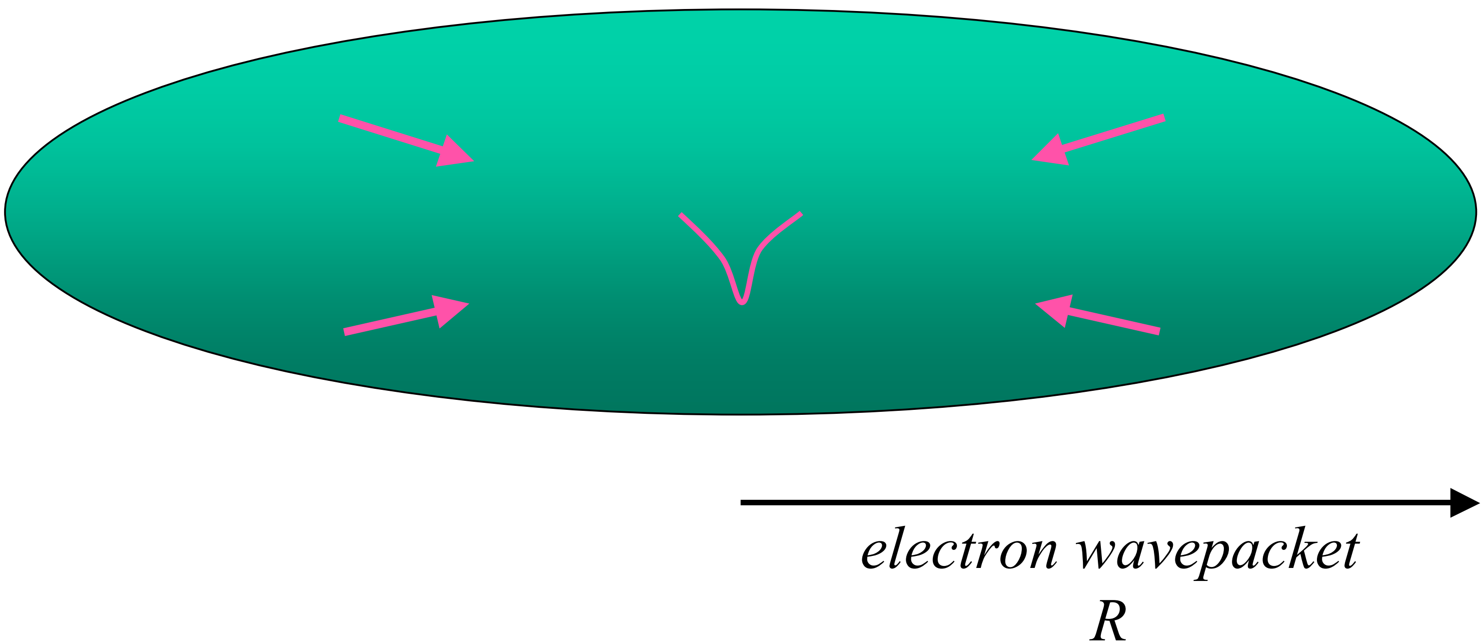
hole in an antiferromagnet (htc)



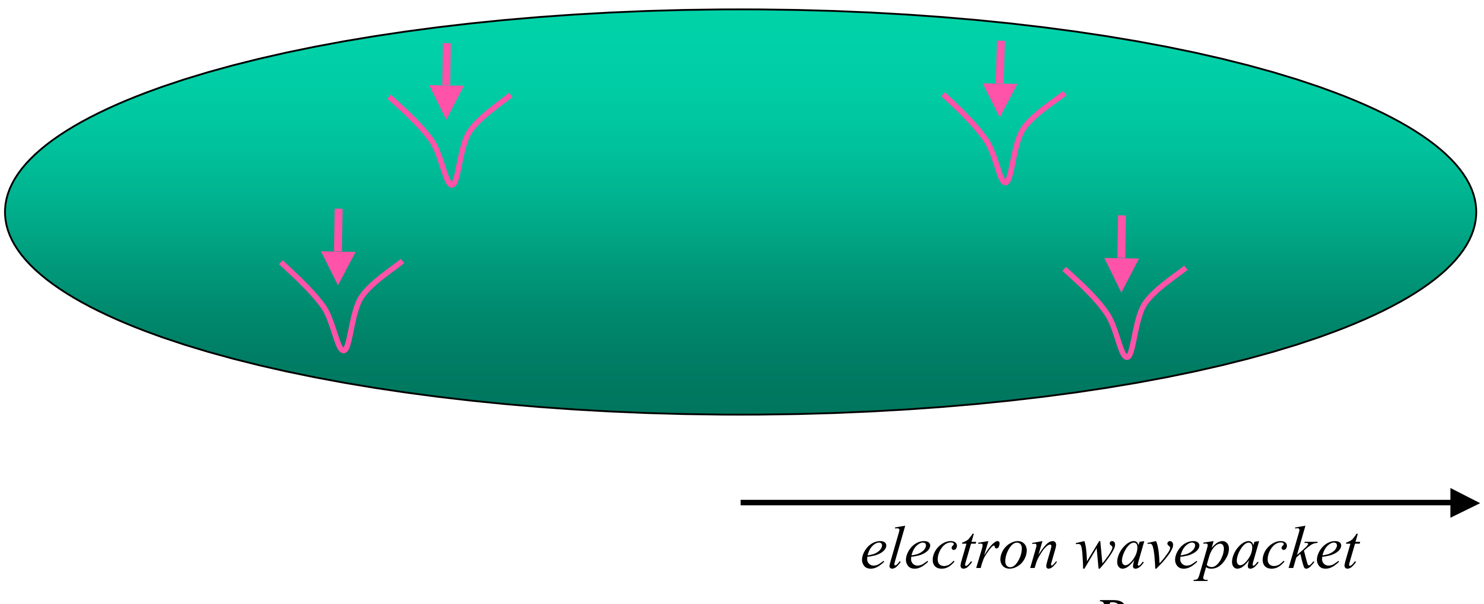




BO / classical phonons



quantum phonons, exact



Semiclassical gives wrong answer: says electron never traps to form a polaron if initial wavepacket is wide.

Why?

BO / semiclassical:
what are the phonons doing?
exact QM:
what are the phonons doing if the electron is on site 1?
what are the phonons doing if the electron is on site 2?
…

semiclassical: 1/N of an electron on each site.
quantum mechanics: full electron on one of the N sites.