Boson-Controlled Quantum Transport

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Topic: Quantum particle strongly interacting with a correlated/fluctuating background medium

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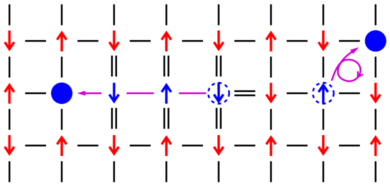
in many cases motion bears resemblance to the “Echternacher Springprozession” ☺

related publication: A. Alvermann, D. M. Edwards, HF, Phys. Rev. Lett. **88**, 056602 ('07)

Gordon Godfrey Workshop on Strong Electron Correlations
UNSW, Sydney, 2007

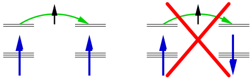
Motivation I

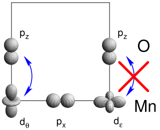
- Strongly correlated charge transport in doped Mott insulators:
  - high-T_c cuprates (AFM spin background)



classical spins: "string effect"
hole is bound to its starting point
quantum spins: "fluctuations"
spin lattice can heal itself with rate controlled by exchange parameter
$\rightsquigarrow$ $t - J-$ type models

  - colossal magnetoresistive manganites (FM spin background)





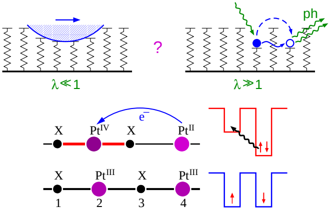
strong Hund's rule coupling
$\rightsquigarrow$ double-exchange model

in addition: orbital anisotropy of hopping & EP (JT) coupling

Spin/orbital degrees of freedom might be represented by (e.g. Schwinger) bosons!

Motivation II

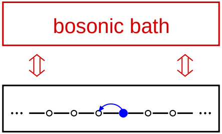
- Charge transport in systems coupled to phonon or bath degrees of freedom
  - polarons/excitons, also in CDW materials, DNA,... (deformable lattice)



polaron motion - diagonal *vs* nondiagonal transitions (band *vs* hopping transport)

$\rightsquigarrow$ Holstein-, Fröhlich-, SSH- or Peierls-Hubbard-type models

  - low-D systems – nanowires, quantum dots (disorder, phonons, $T > 0$)



system, contacts/leads, bath,...

appropriate "microscopic" description/modelling?

Again the transport is strongly boson affected, maybe even fluctuation-induced, but now the correlations within the "background" might be weak or even absent!

Model Hamiltonian I

How to capture this great variety of transport phenomena in a simplified model?

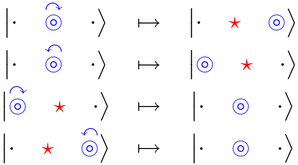
Let's consider the following rather general (spinless!) Hamiltonian:

$$H = -t_b \sum_{\langle i,j \rangle} c_j^\dagger c_i (b_i^\dagger + b_j) - \lambda \sum_i (b_i^\dagger + b_i) + \omega_0 \sum_i b_i^\dagger b_i + \frac{N\lambda^2}{\omega_0}$$

hopping   boson relaxation   boson energy

Electron emits or absorbs a local boson every time it hops between lattice sites [but hopping creates (destroys) a boson only on the site the particle leaves (enters)!]:

$$R_i = c_{i+1}^\dagger c_i b_i^\dagger$$
$$L_i = c_{i-1}^\dagger c_i b_i^\dagger$$
$$L_i^\dagger = c_i^\dagger c_{i-1} b_i$$
$$R_i^\dagger = c_i^\dagger c_{i+1} b_i$$



- $\lambda = 0$ – model is analogous to the classical spin model $\rightsquigarrow$ "string effect"?
- $\lambda > 0$ allows a boson to decay spontaneously $\rightsquigarrow$ healing of the "spin lattice"

Model Hamiltonian II

- Note that "$R_i^{(6)} = L_{i+2}^\dagger L_{i+1}^\dagger R_i^\dagger L_{i+2} R_{i+1} R_i$" acts as "$c_{i+2}^\dagger c_i$":

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$\rightsquigarrow$ lowest order vacuum-restoring process: 1D analogue of 2D "Trugman path"!

- Unitary transformation $b_i \mapsto b_i + t_f/2t_b$ of H

$$H' = -t_f \sum_{\langle i,j\rangle} c_j^\dagger c_i \; - t_b \sum_{\langle i,j\rangle} c_j^\dagger c_i (b_i^\dagger + b_j) \; + \omega_0 \sum_i b_i^\dagger b_i$$

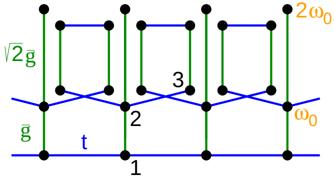
- Different from the t-J model physics of $H^{(')}$ is governed by *two* energy ratios: t_b/t_f and t_b/ω_0, where $t_f = 2\lambda t_b/\omega_0$!

Obviously H' (H) captures the interplay of "coherent" and "incoherent" transport channels realized in many condensed matter systems!

Numerical solution

What does it mean: "Solution"?

- Ground state properties
  Adapt variational Hilbert space construction developed for the Holstein/JT polaron problem (see, e.g., Ku, Trugman, Bonča: PRB 65, 174306 ('02)):



$|1\rangle$ e^- at site 0 with no phonon excitation
$|2\rangle$ e^- and phonon at site 0
$|3\rangle$ e^- at site 1 and one phonon at site 0

i.e., vertical bonds create or destroy phonons

act m times with off-diagonal terms + all translations on an infinite lattice

One- (two-) particle sector: In most cases 10^4-10^6 basis states are sufficient to obtain an *8-16 digit accuracy* for E_0, $\langle 0|\ldots|0\rangle$, ... in *any* dimension! Note that E_0 calculated this way is *variational* for the *infinite* system!

- Spectral properties at T=0, thermodynamics, bath degrees of freedom,...
  Employ Kernel Polynomial Method designed for high-resolution applications: resolution $\propto$ 1/number of moments! (cf. review WWAF: RMP **78**, 275 ('06))
  Chebyshev Space Method – Alvermann, HF: arXiv:0709.3583 [cond-mat.str-el]

Physical quantities of interest

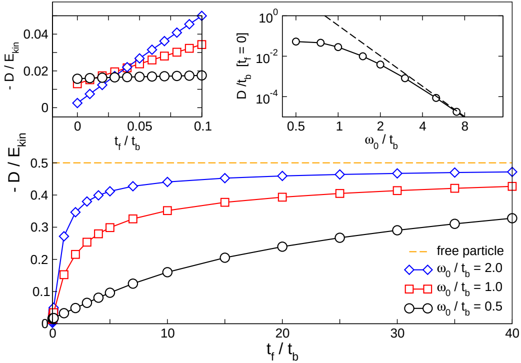
- ground state energy E_0, kinetic energy part $E_{kin} = \langle 0|H - \omega_0 \sum_i b_i^\dagger b_i|0\rangle$
- quasiparticle band dispersion $E(k)$, effective mass $1/m^* = \frac{\partial^2 E(k)}{\partial k^2}|_{k=0}$
- particle-boson correlation function $\chi_{ij} = \langle 0|b_i^\dagger b_i c_j^\dagger c_j|0\rangle$
- one-particle spectral function $A(k,\omega) = \sum_n |\langle n|c_k^\dagger|vac\rangle|^2 \,\delta[\omega - \omega_n]$
- optical conductivity $\mathrm{Re}\sigma(\omega) = 2\pi D\,\delta(\omega) + \sigma_{reg}(\omega)$,

  regular part $\sigma_{reg}(\omega) = \pi \sum_{n>0} \frac{|\langle n|j|0\rangle|^2}{\omega_n} \left[\delta(\omega - \omega_n) + \delta(\omega + \omega_n)\right]$,

  where $j = j_f + j_b$ with $j_f = it_f \sum_i c_{i+1}^\dagger c_i - c_i^\dagger c_{i+1}$
  $j_b = it_b \sum_i c_{i+1}^\dagger c_i b_i^\dagger - c_i^\dagger c_{i+1} b_i - c_{i-1}^\dagger c_i b_i^\dagger + c_i^\dagger c_{i-1} b_i$
- f-sum rule: $\int_{-\infty}^{\infty} \sigma(\omega) d\omega = 2\pi D + 2\int_0^\infty \sigma_{reg}(\omega) d\omega = -\pi E_{kin}$

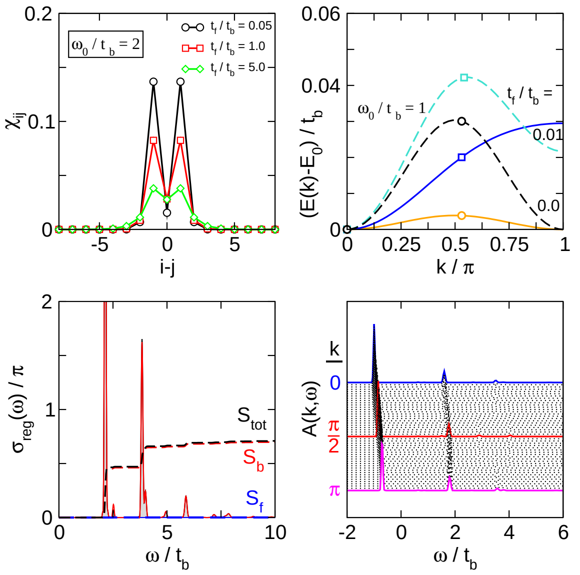
  $\rightsquigarrow$ consistency check: Drude weight $D = 1/2m^*$ (Kohn's formula) ✓

- D scaled to the kinetic energy:



- free particle: $t_b = 0 \rightsquigarrow D = t_f$, i.e., $-D/E_{kin} = 0.5$
- weight of lowest order (vacuum restoring) process scales as t_b^6/ω_0^5
  $\rightsquigarrow$ boson assisted transport dominates for large $(t_b/\omega_0)^5(t_b/t_f)$
- D at $t_f = 0$ saturates for $\omega_0 \to 0$

Correlation-dominated regime



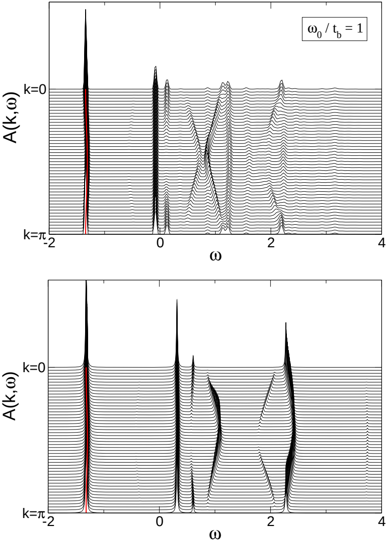
$t_f \leqslant t_b$ (ω_0 not too small):

- pronounced NN particle-boson correlations
- strongly renormalised but well-defined quasiparticle band (reminiscent of spin polaron in the t-J model)

- optical response - threshold given by ω_0
- $\sigma^{reg} \simeq \sigma_b^{reg}$
  $S_{tot}(\omega) = \int_0^\omega \sigma^{reg}(\omega')d\omega'$
- $A(k,\omega)$ signals coherent transport

$\rightsquigarrow$ "collective" particle-boson dynamics!

LIMIT $t_f = 0$ $(\lambda = 0)$



- exact numerical solution

  – particle is still itinerant (but D is small)

  – incoherent contributions

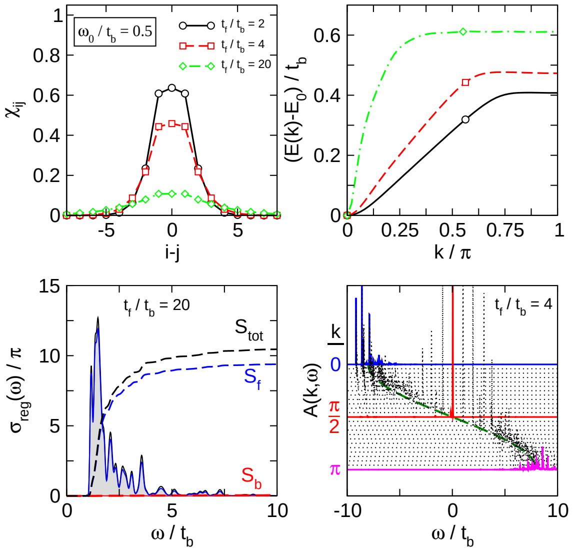
  – $k \to k + \pi$ symmetry

- m-boson analytical solution

Green function decomposition technique $\rightsquigarrow$ (matrix) continued fraction representation

$m \leqslant 3$ exact solution possible; only a finite number of states is accessible for the infinite system

$m \geqslant 4$ infinitely many states will survive



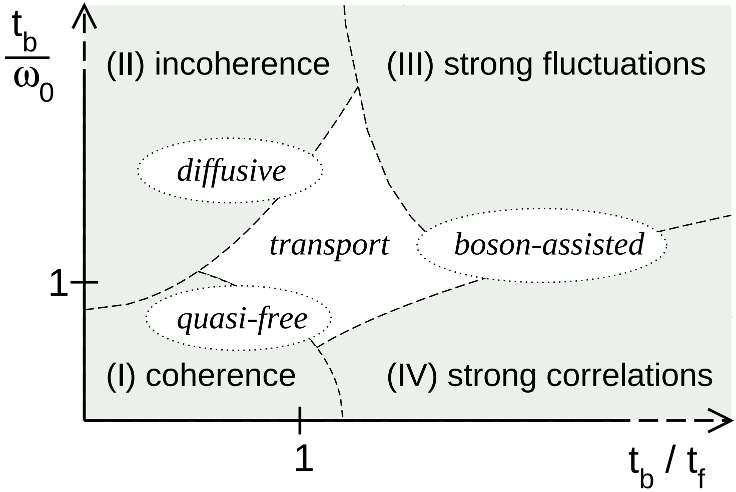
$t_f \gg t_b$ (ω_0 rather small):

- bosons form a cloud around the particle but are not further correlated
- band flattening near the Brillouin zone boundary

  Both is reminiscent of large lattice polarons e.g. in the Holstein model!

- optical response - broad absorption feature
- overdamped character of $A(k,\omega)$ near $k = 0, \pi$
- system is almost transparent at $k = \pi/2$

$\rightsquigarrow$ "diffusive" transport!



t_b / ω_0
(II) incoherence
(III) strong fluctuations
diffusive
transport
boson-assisted
1
quasi-free
(I) coherence
(IV) strong correlations
1
t_b / t_f

Subsumption – One-particle sector

The model that we propose provides a reduced but realistic description of fundamental aspects of transport in the presence of bosonic fluctuations.

Exact numerical solution $(N \to \infty) \rightsquigarrow$ surprisingly rich physics:

- moving particle creates local distortions of substantial energy in the medium, which may be able to relax
- their relaxation rate determines how fast the particle can move
- "free" particle $\leftrightharpoons$ magnetic polaron $\leftrightharpoons$ lattice polaron
- coherent (correlated) $\leftrightharpoons$ incoherent (diffusive) transport
- bosonic fluctuations act in two competing ways:
  limit transport & assist transport!

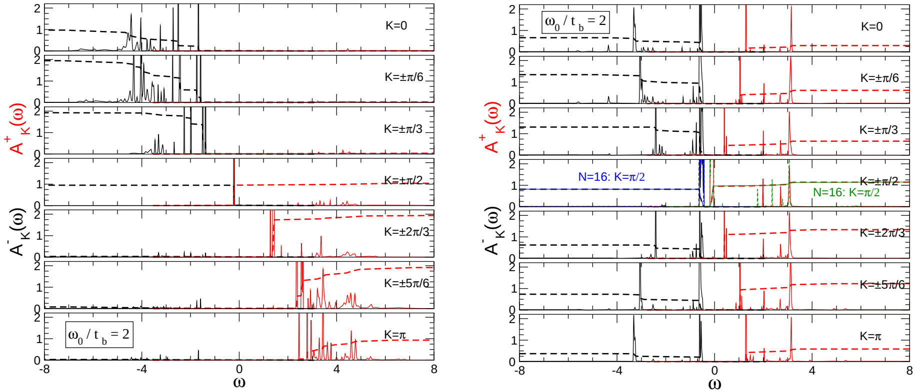
And all this is obtained for just one particle! Plus background! ☺

What about finite carrier density? Half-filled band case? Quantum phase transitions?

- (Inverse) Photoemission spectra (large-scale ED results – $N = 12 \ldots 16$; PBC)

correlation-dominated regime: $\omega_0/t_b = 2$

$\lambda = 1\ (t_f/t_b = 1)$ $\lambda = 0.01\ (t_f/t_b = 0.01)$

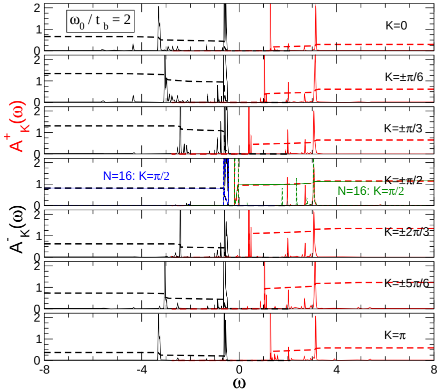


▶ MIT takes place as λ (or t_f) $\searrow$ at fixed ω_0 !

Band Structure

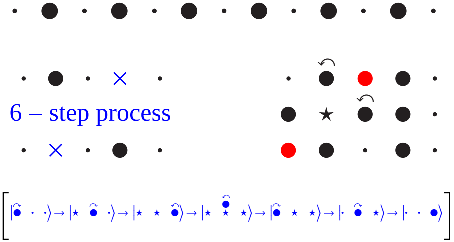
- Doping the insulating state...

$\lambda = 0.01 \; (t_f/t_b = 0.01)$



flat (lower) - dispersive (upper) band

dominant hopping processes starting from an AB structure:



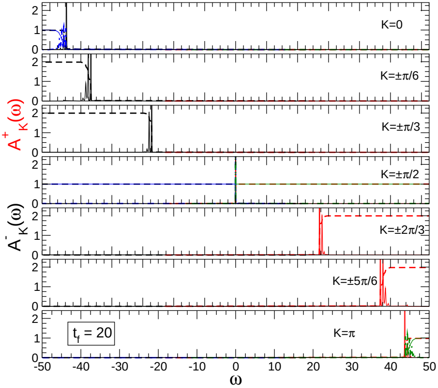
▶ correlation-dominated regime $\rightsquigarrow$ asymmetric "band structure"

Metal insulator transition II

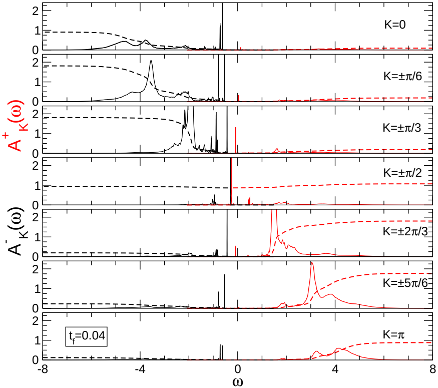
- Fluctuation-dominated regime?

$\omega_0 / t_b = 0.5$

$\lambda = 5$



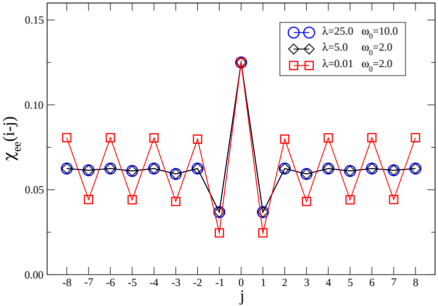
$\lambda = 0.01$

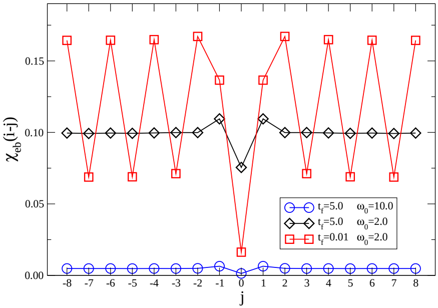


▶ MIT is suppressed as $\omega_0 \searrow$ at fixed λ !

- Particle-particle and particle-boson correlation functions?

$$\chi_{ee}(i-j) = \frac{1}{N_e^2} \sum_i \langle n_i n_{i+j} \rangle \qquad \chi_{eb}(i-j) = \frac{1}{N_e} \sum_i \langle n_i b_{i+j}^\dagger \rangle$$





▶ at the MIT long-range order develops !

Summary – Open problems

We studied the interplay of collective dynamics and damping in the presence of correlations and fluctuations within a two-channel transport model.

The newly proposed model covers basic aspects of very different Hamiltonians: Hubbard, $t-J$ . . . , Fröhlich, Holstein, . . . , SSH - type.

- Influence of spatial dimensionality? VED ✓
- What about two particles - binding? VED ✓
- Finite-density effects ($0 \leqslant n \leqslant 1$)? DMRG (✓)
- Finite-temperature effects? QMC ?
- Different lattice structures? Frustration! ?
- We need a better analytical understanding of the model, maybe at least for some important limiting cases!

  [1D, $\lambda = 0$ & 3-4 boson approximation,. . . , semiclassical limit (?),. . .]

Everybody is invited to contribute...

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