Correlation-induced metal-insulator transition in a two-channel fermion-boson model:

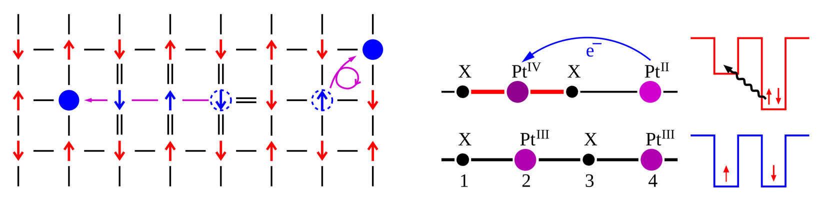
Luttinger liquid versus charge-density-wave behavior

H. Fehske†, S. Ejima†, A. Alvermann†, G. Hager*, G. Wellein* and D. M. Edwards‡

†Universität Greifswald, *Universität Erlangen-Nürnberg, ‡Imperial College London

Motivation

The motion of a particle that interacts strongly with some background medium is a constantly recurring theme in condensed matter physics. Media which commonly occur are ordered spin backgrounds as in the t-J model of doped Mott insulators, or vibrating lattices as in the Holstein or quantised SSH models for polarons or charge density waves (CDW).



Quantum transport in correlated/fluctuating background media like 2D AFM (high-T_c cuprates) or 1D CDW (MX chains).

Note that in all cases transport is strongly boson affected or even controlled because as the particle moves it creates local distortions of substantial energy in the medium, e.g. local spin or lattice fluctuations, which may be able to relax. Their relaxation rate determines how fast the particle can move. The interaction with the background may even drive a metal insulator transition (MIT). The proof of existence of MIT in generic model Hamiltonians is one of the most fundamental problems in solid state theory. As yet there is only a very small number of microscopic models which have rigorously been shown to exhibit a MIT.

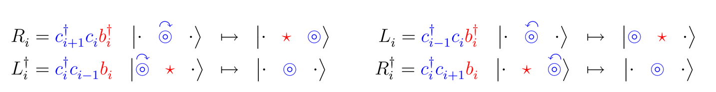
Model

To model these principal transport mechanisms a rather simple (spinless) Hamiltonian with a novel form of fermion-boson coupling has recently been proposed (*D. M. Edwards, Physica 378-380B, 133 (2006)*):

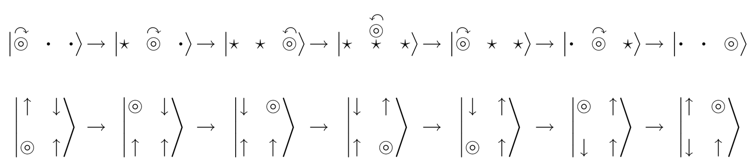
$$H = -t_b \sum_{\langle i,j\rangle} c_j^\dagger c_i (b_i^\dagger + b_j) - \lambda \sum_i (b_i^\dagger + b_i) + \omega_0 \sum_i b_i^\dagger b_i$$

hopping + boson relaxation + boson energy

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



The λ term allows a boson to decay spontaneously, thereby avoiding the string effect (compare λ with J). Thus t-J-like quasiparticle transport becomes possible. However, even at $\lambda = 0$, when transport is fully boson-assisted, there exist processes that propagate the particle but restore the boson vacuum. The lowest-order process of this kind comprises 6 steps: "$R_i^{(6)} = L_{i+2}^\dagger L_{i+1}^\dagger R_i^\dagger L_{i+2} R_{i+1} R_i$" acts as "$c_{i+2}^\dagger c_i$"!



⇝ 1D analogue of 2D "Trugman paths"!

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 $H' = H_f + H_b + H_{\omega_0}$ 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 Methods

Ground state properties

Single-particle sector: Variational Hilbert space approach *(Ku, Trugman, Bonča: PRB 65, 174306 (2002))*. In most cases 10^6 basis states are sufficient to obtain an 8-16 digit accuracy for E_0, $\langle 0|\ldots|0\rangle$, ... in *any* dimension!

Many-particle sector: DMRG pseudo-site approach *(see, e.g. Jeckelmann, Fehske, Rivista del Nuovo Cimento 30, 259 (2007))*. We keep $m = 1200$ to 2000 density-matrix eigenstates and extrapolate various quantities to the $m \to \infty$ limit. The discarded weight was always smaller than 5×10^{-8}.

Spectral properties

Kernel Polynomial Method *(Weiße, Wellein, Alvermann, Fehske, RMP 78, 275 (2006))*:

$$A^O(x) = \frac{1}{\pi\sqrt{1-x^2}} \left(\mu_0^O + 2\sum_{m=1}^M \mu_m^O T_m(x) \right)$$

$$\mu_m^O = \int_{-1}^1 dx\, T_m(x) A^O(x) = \langle \psi_0 | O^\dagger T_m(X) O | \psi_0 \rangle .$$

with Chebyshev polynomials $T_m(x) = \cos[m \arccos(x)]$ and moments $\mu_{2m}^O = 2\langle \phi_m|\phi_m\rangle - \mu_0^O$, $\mu_{2m+1}^O = 2\langle \phi_{m+1}|\phi_m\rangle - \mu_1^O$.

Single-Particle Sector

(Alvermann, Edwards, Fehske, PRL 98, 056602 (2007))

♣ *Drude weight - f-sum rule*

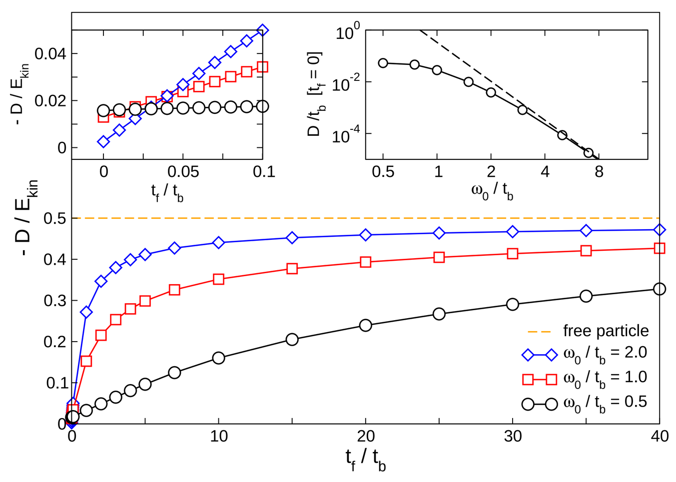
$$-D = \frac{E_{kin}}{2} + \int_0^\infty \sigma_{reg}(\omega) d\omega$$

♣ *optical conductivity*

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

(here $j = j_f + j_b$ with $j_f = \mathrm{i}t_f \sum_i c_{i+1}^\dagger c_i - c_i^\dagger c_{i+1}$, $j_b = \mathrm{i}t_b \sum_i c_{i+1}^\dagger c_i b_i^\dagger - c_i^\dagger c_{i+1} b_i - c_{i-1}^\dagger c_i b_i^\dagger + c_i^\dagger c_{i-1} b_i$)

♣ *Kohn's formula* $D = 1/2m^*$ ⇝ consistency check!



D (scaled to E_{kin}) as a function of t_f/t_b. The dashed curve gives the asymptotic result $D \simeq t_b^6/(3\omega_0^5) + O(t_b^8/\omega_0^7)$ for $\omega_0 \to \infty$.

- free particle ($t_b = 0$): $D = t_f$, $-D/E_{kin} = 0.5$
- strong fluctuations: $-D/E_{kin} \ll 0.5$ ⇝ diffusive transport
- strong correlations: $D \nearrow$ as $\omega_0 \searrow$ (see inset) ⇝ boson-assisted hopping – transport dominated by vacuum-restoring (6-step) processes

♣ *particle-boson & particle-particle correlations*

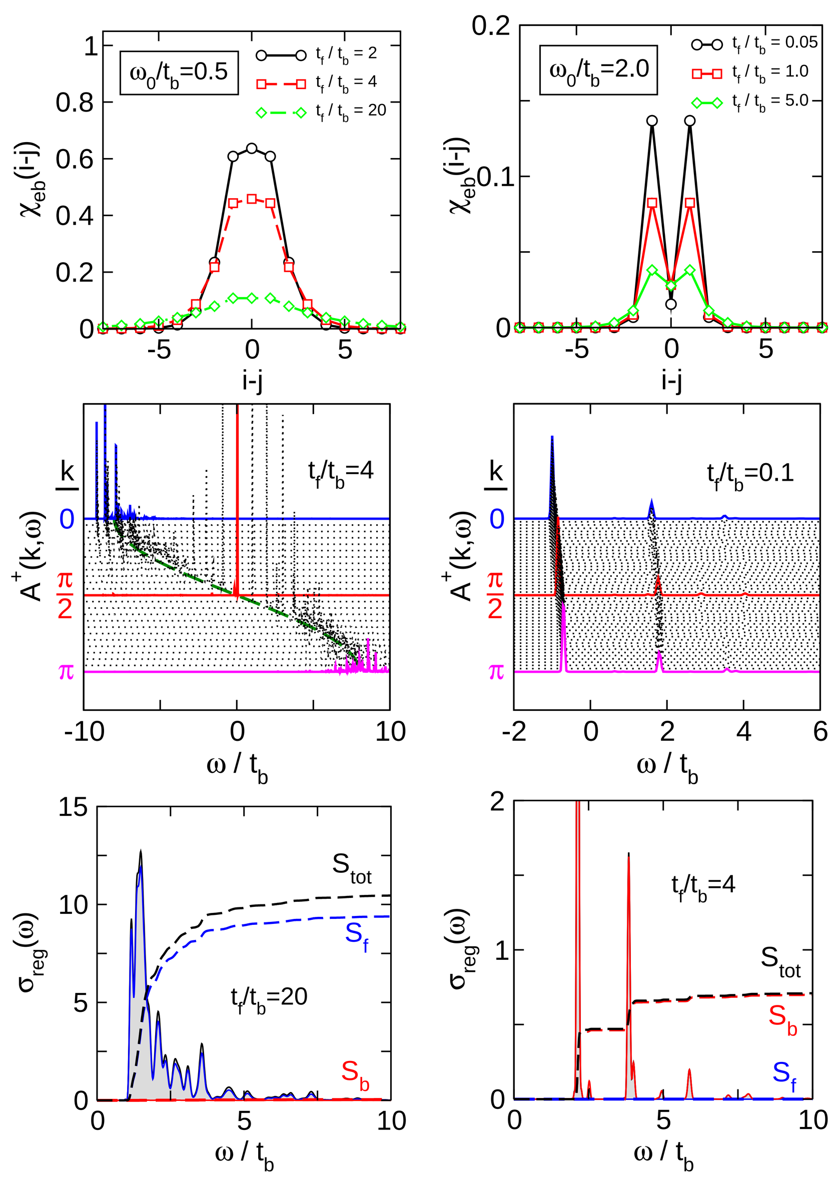
$$\chi_{eb}(i-j) = \frac{1}{N_e} \sum_i \langle \psi_0 | c_i^\dagger c_i b_{i+j}^\dagger b_{i+j} | \psi_0 \rangle$$

$$\chi_{ee}(i-j) = \frac{1}{N_e^2} \sum_i \langle \psi_0 | c_i^\dagger c_i c_{i+j}^\dagger c_{i+j} | \psi_0 \rangle$$

♣ *single-particle excitations related to photoemission (PE) $A^-(k,\omega)$ and IPE $A^+(k,\omega)$ processes*

$$A^\pm(k,\omega) = \sum_n |\langle \psi_n^\pm | c_k^\pm | \psi_0 \rangle|^2 \delta[\omega \mp \omega_n^\pm]$$

(here $c_k^+ = c_k^\dagger$, $c_k^- = c_k$, $|\psi_0\rangle$ is the ground state in the N_e-particle sector while $|\psi_n^\pm\rangle$ denote the n-th excited states in the $N_e \pm 1$-particle sectors with $\omega_n^\pm = E_n^\pm - E_0$)



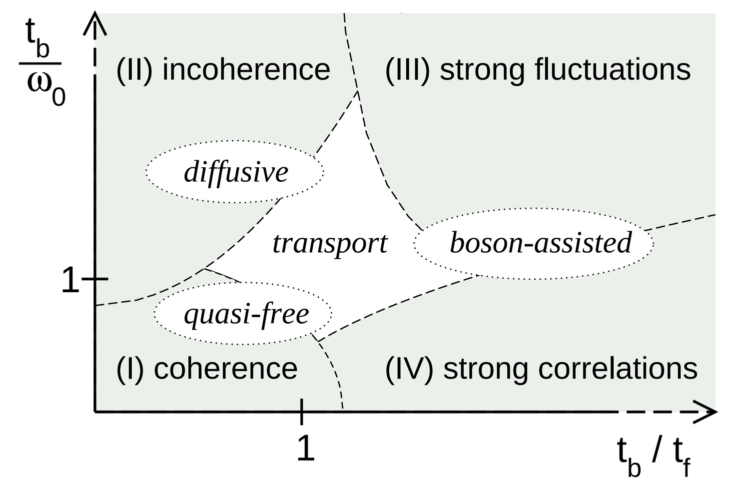
Electron-boson correlations $\chi_{eb}(i-j)$, spectral function $A^+(k,\omega)$, and optical response $\sigma_{reg}(\omega)$ (from top to bottom). Left (right) column gives data for $\omega_0/t_b = 0.5$ ($\omega_0/t_b = 2.0$), i.e. in the fluctuation (correlation) dominated regime. S_{tot} denotes the integrated conductivity $S_{tot}(\omega) = \int_0^\omega \sigma_{reg}(\omega')d\omega'$.

• $t_f \gg t_b$ (ω_0 rather small) ⇝ "diffusive" transport!

- bosons form a cloud around the particle
- band flattening near the Brillouin zone boundary
- optical response - broad absorption feature
- overdamped character of $A(k,\omega)$ near $k = 0, \pi$

• $t_f \le t_b$ (ω_0 not too small) ⇝ "collective" particle-boson dynamics!

- pronounced NN particle-boson correlations
- optical response - threshold ω_0; $\sigma_{reg} \simeq \sigma_{reg,b}$
- $A(k,\omega)$ signals coherent transport within a strongly renormalised quasiparticle band



Schematic "phase diagram" of our transport model.

Exact numerical solution ($N \to \infty$) ⇝ surprisingly rich physics: "free" particle ⇆ magnetic polaron ⇆ lattice polaron; coherent (correlated) ⇆ incoherent (diffusive) transport. Bosonic fluctuations act in two competing ways: limit transport & assist transport!

All this is obtained for just one particle - plus background!

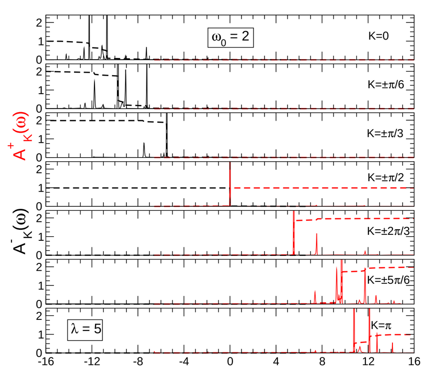
Half-filled Band Case

Spectral properties – ED/KPM

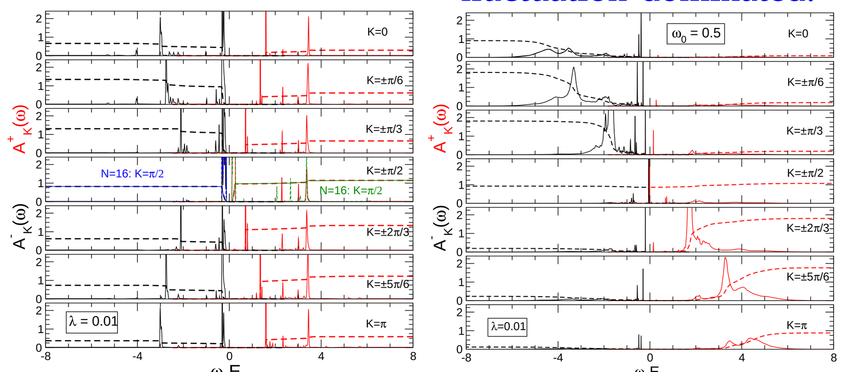
(Wellein, Fehske, Alvermann, Edwards, PRL 101, 135402 (2008))

Does our boson-controlled hopping model shows a metal insulator QPT at commensurate band fillings? Since the particles have only a charge degree of freedom, the formation of a CDW is the only possibility for a MIT. Clearly the free hopping channel ($\propto t_f$) acts against any correlation induced CDW, but also strong bosonic fluctuations will destroy LRO.

♣ *wave-vector resolved single-particle spectra* ($D_{tot}^{max} \simeq 8 \times 10^{10}$, 30 000 CPUh per spectrum)

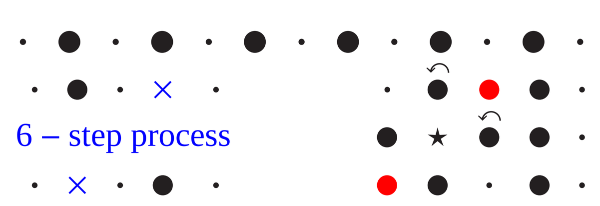


correlation-dominated: fluctuation-dominated:



PE (black) and IPE spectra (red) for the half-filled band case with $\lambda = 5$ [$t_f(\lambda, \omega_0 = 2) = 5$] (upper panel) and $\lambda = 0.01$ (lower panels), where $\omega_0 = 2$ [$t_f(\lambda, \omega_0) = 0.01$] (left) or $\omega_0 = 0.5$ [$t_f(\lambda, \omega_0 = 2) = 0.04$] (right), for $N = 12$, $N_b = 15$. Dashed lines give $S_K^\pm(\omega - E_F) = \int_0^\omega d\omega' A_K^\pm(\omega' - E_F)$, where $S_K = S_K^-(-\infty) + S_K^+(\infty) = 1$, and $\sum_K S_K = N$. (ω is rescaled with respect to E_F; energies measured in units of $t_b = 1$; PBC).

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



States with one particle removed from a perfect CDW (left panel) are connected by the 6-step hopping process of order $\mathcal{O}(t_b^6/\omega_0^5)$, whereas a 2-step process of order $\mathcal{O}(t_b^2/\omega_0)$ (right panel) relates states with an additional particle. Consequently the electron band is much less renormalised than the hole band, and the mass enhancement is by a factor $\mathcal{O}((t_b/\omega_0)^4)$ smaller.

Correlation induced mass-asymmetric band structure, different in nature from simple 2-band models!

⇝ MIT is suppressed as ω_0 decreases (i.e. fluctuations increase) at fixed λ !

Ground-state properties – DMRG

(Ejima, Hager, Fehske, PRL 102, 106404 (2009))

In order to characterize the metallic and insulating regimes in more detail we calculate besides the local particle densities and fermion-boson correlation functions, the

♣ *kinetic energy parts*

$$E_{b/f}^{kin} = \langle \psi_0 | H_{b/f} | \psi_0 \rangle ,$$

♣ *charge structure factor*

$$S_c(q) = \frac{1}{N} \sum_{j,l} e^{iq(j-l)} \left\langle \left(c_j^\dagger c_j - \frac{1}{2} \right) \left(c_l^\dagger c_l - \frac{1}{2} \right) \right\rangle ,$$

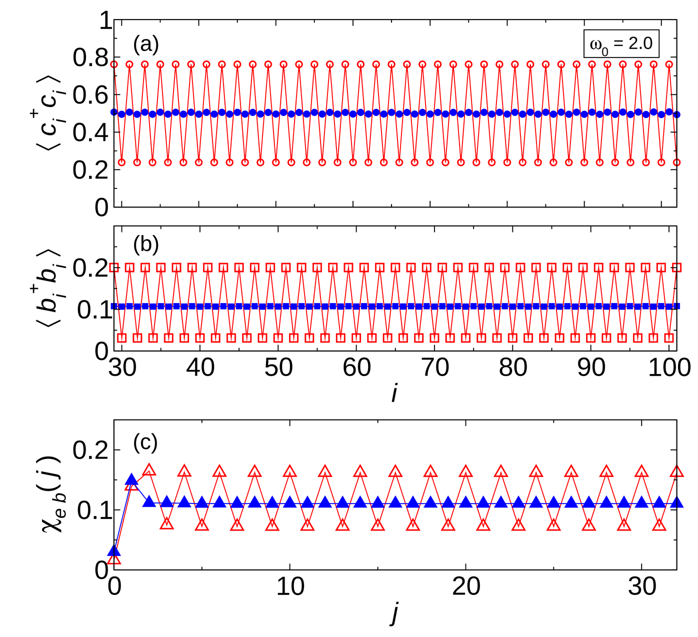
♣ *Luttinger liquid charge exponent*

$$K_\rho = \pi \lim_{q \to 0} \frac{S_c(q)}{q}, \quad q = \frac{2\pi}{N}, \quad N \to \infty ,$$

♣ *single-particle (charge) excitation gap*

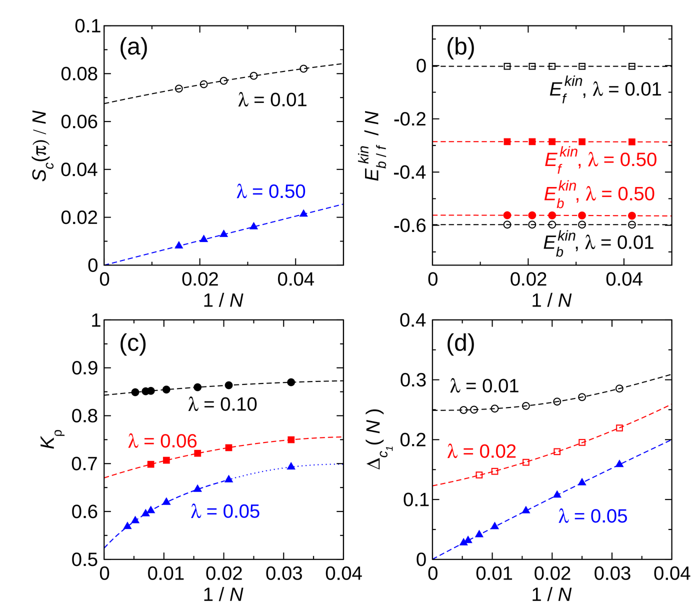
$$\Delta_{c_1}(N) = E(N_e + 1) + E(N_e - 1) - 2E(N_e),$$

where $E(N_e)$ and $E(N_e \pm 1)$ are the ground-state energies in the N_e and $(N_e \pm 1)$ particle sectors, respectively, with $N_e = N/2$.



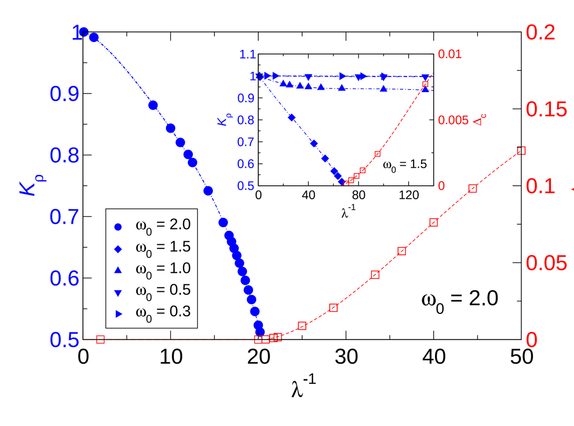
Local densities of fermions $\langle c_i^\dagger c_i \rangle$ (a) and bosons $\langle b_i^\dagger b_i \rangle$ (b) for a 128-site system with OBC. Open symbols are for $\lambda = 0.01$ (CDW regime), filled ones for $\lambda = 0.5$ (metallic regime). The fermion-boson correlation function $\chi_{eb}(j)$ is given in panel (c) for a 64-site system with APBC (discarded weight 1.4×10^{-10} (7.9×10^{-10}) for $\lambda = 0.01$ ($\lambda = 0.50$)). In all cases $\omega_0 = 2.0$.

- CDW structure of the insulating state shows up in the local densities and fermion-boson correlations
- metallic regime: OBC ⇝ Friedel oscillations (which algebraically decay → interior)



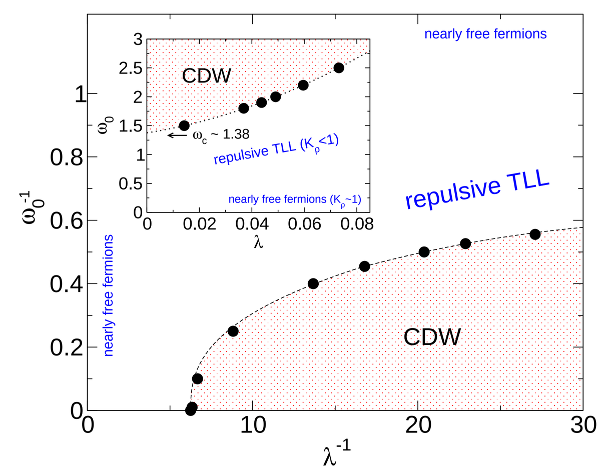
Finite-size scaling of several physical quantities: (a) static charge structure factor $S_c(q)$ at $q = \pi$, (b) kinetic energy parts $E_{b/f}^{kin}$, (c) Luttinger liquid parameter K_ρ, and (d) single-particle excitation gap Δ_{c_1}. Data obtained for $\omega_0 = 2$ with APBC [(a),(b)] and OBC [(c),(d)] applied.

- $\lambda = 0.01$, $\omega_0 = 2$: $S_c(\pi)/N$ stays finite in the thermodynamic limit ⇝ true CDW long-range order



$N \to \infty$ extrapolated values of the single-particle gap Δ_{c_1} (squares) and TLL parameter K_ρ as a function of λ^{-1} for $\omega_0 = 2.0$ (main panel). The inset displays results for smaller ω_0 and shows that (i) no CDW state is found for $\omega_0 < \omega_c$ and (ii) $K_\rho < 1$ for all ω_0, where $K_\rho \to 1$ as $\omega_0 \to 0$ and/or $\lambda^{-1} \to 0$.

- Lowering λ, K_ρ decreases from $1 \to 1/2$. The point where $K_\rho = 1/2$ is reached marks the critical coupling for the MIT.



DMRG phase diagram for the 1D half-filled band case. The inset gives the phase diagram in the λ-ω_0 plane. The MIT point for $\lambda = 0$, $\omega_0(0) \sim 1.38$, is obtained from a quadratic fit.

- TLL exists even for $\omega_0 = \infty$ provided that $\lambda^{-1} < \lambda_c^{-1}(\omega_0 = \infty) \simeq 6.3$
- TLL is realized for $\lambda = 0$ below $\omega_c \simeq 1.38$

To conclude, using unbiased numerical techniques, we proved that our very two-channel fermion-boson transport model displays a correlation-induced MIT at half filling in 1D. The metallic phase typifies a repulsive Luttinger liquid, while the insulating phase shows CDW long-range order. The CDW ground state is a few-boson state, in contrast e.g. to a dimerized Peierls phase.