One-Dimensional Quantum Transport Affected by a Background Medium: Fluctuations versus Correlations

S. Ejima and H. Fehske
Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, 17489 Greifswald, Germany

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We analyze the spectral properties of a very general two-channel fermion-boson transport model in the insulating and metallic regimes, and the signatures of the metal-insulator quantum phase transition in between. To this end we determine the single particle spectral function related to angle-resolved photoemission spectroscopy, the momentum distribution function, the Drude weight and the optical response by means of a dynamical (pseudo-site) density-matrix renormalization group technique for the one-dimensional half-filled band case. We show how the interplay of correlations and fluctuations in the background medium controls the charge dynamics of the system, which is a fundamental problem in a great variety of advanced materials.

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I. INTRODUCTION

Charge transport normally takes place in some background medium. To understand how the environment affects the moving carrier and vice versa is a difficult question and in this generality at present perhaps one of the most heavily debated issues in condensed matter physics. Here the term “background” describes a variety of situations. We can think of the motion of a hole through an ordered insulator. Examples are the high-\(Tc\) cuprates and the colossal magnetoresistive manganates, with a background of spins and orbitals, respectively, forming a pattern of alternating order. Then, as the hole moves, it disrupts the order of the background, which on its part hinders the particle transfer. Nevertheless coherent particle transport may occur, but on a strongly renormalized energy scale. The new quasiparticles formed in the cuprates and manganates are spin or orbital polarons\cite{1,2,3,4}. Another situation concerns a charge carrier coupled to a deformable background. Here, if the interaction with phonons is strong, the particle has to carry a phonon cloud through the medium. The outcome might be a “self-trapped” small lattice polaron\cite{5}. In this case hopping transport, accompanied by phonon emission and absorption processes, evolves as the dominant transport channel.

So far we have considered a single particle only. It is quite obvious that the problem becomes even more involved if the particle density increases. Then the interrelation between charge carriers and background medium may drive quantum phase transitions. The appearance of ferromagnetism in the three-dimensional (3D) manganates, superconductivity in the quasi-2D cuprates, or charge-density-wave (CDW) states in 1D halogen-bridged transition metal complexes are prominent examples\cite{5,6,7,8}. In the theoretical description of these strongly correlated systems an additional difficulty arises: The particles which are responsible for charge transport and the order phenomena of the background are the same. As a consequence, on a microscopic level, rather involved many-particle models result, which incorporate the coupling between charge, spin, orbital and lattice degrees of freedom\cite{9,10}. Naturally this prevents an exact solution of the problem even in reduced dimensions.

II. MODEL AND METHOD

A way out might be the construction of simplified transport models, which capture the basic mechanisms of quantum transport in a background medium in an effective way. Along this line a novel quantum transport model has been proposed recently\cite{11,12}.

\[
H = -t_b \sum_{\langle i,j \rangle} f_i^\dagger f_j(b_i^\dagger + b_j) - \lambda \sum_i (b_i^\dagger b_i + b_i b_i^\dagger) + \omega_0 \sum_i b_i^\dagger b_i, \tag{1}
\]

which mimics the correlations inherent to a spinful fermionic many-particle systems by a boson affected hopping of spinless particles \( \propto t_b \) (see Fig. 1). In the model \( \mathcal{H} \), a fermion \( f_i^{(1)} \) creates (or absorbs) a local boson \( b_i^{(1)} \) every time it hops, which corresponds to a local excitation in the background with a certain energy \( \omega_0 \). Because of quantum fluctuations the distortions are able to relax \( \propto \lambda \). A unitary transformation \( b_i \to b_i + \lambda/\omega_0 \) replaces this term by second transport channel \( H_f = -t_f \sum_{\langle i,j \rangle} f_i^\dagger f_j, \) describing unaffected fermionic transfer, however with a renormalized amplitude \( t_f = 2\lambda t_b/\omega_0 \). It has been shown\cite{13} that coherent propagation of a fermion is possible even in the limit \( \lambda = t_f = 0 \) by means of a six-step vacuum-restoring hopping process,

\[
R_i^{(6)} = L_{i+2}^\dagger L_{i+1}^\dagger R_i L_{i+2} R_{i+1} R_i, \tag{2}
\]

where \( R_i^{(6)} = f_i^\dagger f_{i+1} b_i \) and \( L_i^\dagger = f_i^\dagger f_{i-1} b_i \). Note that \( R_i^{(6)} \) acts as direct next nearest neighbor (NNN) transfer \( f_{i+2}^\dagger f_i \), in complete analogy to the “Trugman path” of a hole in a 2D Néel-ordered spin background\cite{14}.

The model \( \mathcal{H} \) has been solved in the single particle sector (\( N_c = 1 \)) by exact diagonalization\cite{15}, using a basis construction for the fermion-boson (many-particle)
Hilbert space that is variational for an infinite lattice ($N = \infty$). The transport behavior was found to be surprisingly complex, reflecting the properties of both spin and lattice polarons in $t$-$J$- and Holstein-type models.

For the 1D half-filled band sector ($N_e = N/2$), evidence for a metal insulator transition comes from small cluster diagonalizations. Quite recently the ground-state phase diagram of the model (1) has been mapped out in the whole $\lambda - \omega_0$ plane, using a density-matrix renormalization group (DMRG) technique. A quantum phase transition of a Tomonaga-Luttinger liquid (TLL) and CDW was proven to exist. A complementary study of the dynamical properties of the system is therefore desirable.

In the present work, we employ the dynamical DMRG (DDMRG) method in order to investigate the effects of background fluctuations and correlations on the dynamics of charge carriers in the framework of the 1D half-filled fermion-boson model (1). Thereby the focus is on the wave-vector resolves single-particle spectral function probed by angle-resolved photoemission spectroscopy (ARPES) and on the optical conductivity probed e.g. by reflectivity measurements.

In general the dynamic response of a quantum system described by a time-independent Hamiltonian $H$ is given by the imaginary part of correlation functions of type

$$A_O(\omega) = \lim_{\eta \to 0} \frac{1}{\pi} \frac{1}{(E_0 + \omega - \eta) + \eta^2} O(\psi_0),$$

where the operator $O$ identifies the physical quantity of interest, $|\psi_0\rangle$ and $E_0$ give the ground-state wave function and energy of $H$. The small $\eta > 0$ shifts the poles of the related Green function $G_0(\omega + i\eta)$ into the complex plane.

Single particle excitations associated with the injection or emission of an electron with wave vector $k$, $A^+(k, \omega)$ or $A^-(k, \omega)$, can be written in the spectral form

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

where $f_k^+ = f_k^\dagger$, $f_k = f_k$ and $|\psi_0\rangle$ is the groundstate of a $N$-site system 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 excitation energies $\omega_n^\pm = E_n^\pm - E_0$.

Optical excitations, on the other hand, connect states in the same particle sector with a site-parity change. For a system with open boundary conditions (OBC) the regular part of the optical absorption is

$$\sigma_{reg}(\omega) = \frac{\pi}{N} \sum_n \omega_n |\langle \psi_n | P | \psi_0 \rangle|^2 \delta[\omega - \omega_n],$$

where $P = - \sum_{j=1}^N j \left( f_j^+ f_j - 1 \right)$ is the dipole operator (in units of $e$), and $\omega_n \equiv (E_n - E_0)$. Then the current operator is obtained from $J = i[H, P]$. Applying periodic boundary conditions (PBC), the optical conductivity can be calculated from

$$\sigma_{reg}(\omega) = \frac{\pi}{N} \sum_n \frac{|\langle \psi_n | J | \psi_0 \rangle|^2}{\omega_n} \delta[\omega - \omega_n].$$

Note that for our fermion-boson model (1), the current operator has two contributions, $J = J_f + J_b$, where

$J_f = i t f \sum_{j} f_{j+1}^+ f_j - f_j^+ f_{j+1}$ and $J_b = i b \sum_{j} f_{j+1}^+ f_j b_j - f_j^+ f_{j+1} b_j + f_j b_{j+1}^+ - f_j^+ b_j - f_j b_{j+1}$.

The f-sum rule

$$S_{reg}(\infty) + \pi D = - \pi E_{kin}/2.$$
connects the frequency-integrated optical response

\[ S_{\text{reg}}(\omega) = \int_0^\pi \sigma_{\text{reg}}(\omega') d\omega' \] to the kinetic energy \( E_{\text{kin}} = \frac{1}{N} \langle 0 | H - \omega_0 \sum_i b_i^\dagger b_i | 0 \rangle \), where the Drude part \( \propto D \) serves as a measure for coherent transport. For OBC, only a \( D \) precursor exists in the metallic region.

In the actual DDMRG calculation of spectral functions the required CPU time increases rapidly with the number of the density-matrix eigenstates \( m \). Since the DDMRG approach is based on a variational principle, \( m \) we first of all have to prepare a good "trial function" for the ground state with as many density-matrix eigenstates as possible. As a rule we keep \( m \approx 500 \) states to obtain the true ground state in the first five DDMRG sweeps and afterwards take \( m \approx 200 \) states for the calculation of the various spectra from \( \lambda = 0 \) with a broadening \( \eta = 0.1 \). In order to save CPU time in the DDMRG runs we take into account just \( n_k = 3 \) pseudosites. In this case the \( n_k \)-th local boson pseudo-site density is smaller than \( 10^{-5} \). Using \( n_k = 4 \) this value can be reduced to \( 10^{-8} \) which leads, however, not to visible change of the spectra because the discarded weight in the DDMRG calculations is \( \sim 10^{-3} \) (i.e. three orders of magnitude larger than for the DMRG ground-state calculations).

### III. RESULTS

#### A. Photoemission spectrum

Let us first discuss the single-particle spectra of the transport model \( \text{[(1)]} \) in the regime where the background is stiff, i.e. the distortions induced by the particle hopping process are energetically costly (\( \omega_0 = 2 \)).

For very large \( \lambda \) the free transport channel nevertheless dominates and an almost particle-hole symmetric spectrum \( (A^+(k, \omega - E_F) \sim A^-(k - \pi, E_F - \omega)) \) results (see Fig. 2 upper panels). As \( \lambda \) decreases, the background distortions hardly relax. Consequently the bosonic degrees of freedom will strongly affect the transport. The middle panels of Fig. 2 show how, at \( \lambda = 0.1 \), strong correlations develop in the occupied states probed by photoemission (PE) for \( \omega < E_F \). The introduced hole can only move coherently by the 6-step process \( \text{[(2)]} \), where in step 1-3 three bosons were excited, which are consumed in steps 4-6 afterwards. In this way the collective particle-boson dynamics leads to a flattening of the "coherent" band for \( k \leq k_F \). By contrast an additional electron, which probes the unoccupied states in an inverse (I)PE experiment (\( \omega > E_F \)), can more easily move by a two-step process, even if pronounced CDW correlations exist in the background medium \( \text{[(3)]} \). The incoherent parts of \( A(k, \omega) \) far away from the Fermi energy \( E_F \) are caused by excitations with additional bosons involved (bear in mind that the ground state with \( N \) electrons is a multi-phonon state and the wave vector of the \( N \) target state corresponds to the total momentum of electrons and bosons).

While for \( \lambda = 0.1 \), \( A(k_F, \omega) \) has finite spectral weight at \( E_F \), i.e. the system is still metallic (albeit the TLL charge exponent \( K_\rho \) is noticeably reduced from one \( \text{[(13)]} \)), an excitation gap opens in the PE spectrum as \( \lambda \) falls below a certain critical value, provided that \( \omega_0 > \omega_0^{\text{CDW}}(\lambda = 0) \text{[(13)]} \). We find \( \lambda_0(\omega_0 = 2) \simeq 0.05 \). The lower panels of Fig. 2 show \( A(k, \omega) \) for \( \lambda = 0.01 \), in the insulating regime, where a CDW with true long-range order exists. The TLL–CDW quantum phase transition is driven by the correlations that might evolve in the background medium at commensurate fillings. Let us emphasize the dynamical aspect of this process: The (collective) bosonic excitations are intimately connected to the motion of the particles, and themselves have to persist long enough in order to affect the many-particle state. The ARPES spectrum for the insulating state clearly shows the doubling of the Brillouin zone. The remaining asymmetry with regard to the spectral weight of the absorption sig-
nals as \( k \rightarrow (\pi - k) \) vanishes for \( \lambda \rightarrow 0 \). Most notably the widths of the highest PE and lowest IPE coherent bands differ by a factor of about \((t_b/\omega_0)^4\), since the CDW order is restored if the injected hole [electron] is transferred to a NNN site by a process of order \( O(t_b^2/\omega_0^5) \). Hence the CDW state exhibits a correlation-induced asymmetric band structure.\(^12\)

The strong interrelation of charge dynamics and background fluctuations becomes obvious if we decrease \( \omega_0 \) below \( \omega_{0,c} \), keeping \( \lambda = 0.01 \) fixed. Of course, in passing the accompanied insulator-metal transition the PE spectrum changes completely, but the “nature” of the TLL at \( \omega_0 = 1 \) is different compared to that of the metallic state realized at larger \( \omega_0 \) and \( \lambda \) as well (cf. Fig. 3 and upper panels of Fig. 2). The single-particle spectrum for \( \omega_0 = 1 \) shows sharp absorption signals in the vicinity of \( k_F \) only. In a wide \( k \)-space region emanating from \( k = 0 \) \((k = \pi)\) the PE (IPE) spectrum is smeared out (over-damped), i.e. here the dynamics of the system is dominated by bosonic fluctuations.

### B. Momentum distribution function

The different transport behavior becomes also apparent in the momentum distribution function

\[
n(k) = \frac{1}{N} \sum_{j,l} e^{i(k\langle j \rangle - l)} \langle c_j^{\dagger} c_l \rangle. \tag{8}\]

By means of DMRG, the ground-state correlation function \( \langle c_j^{\dagger} c_l \rangle \) can be easily calculated for PBC. Figure 4 displays \( n(k) \) for two characteristic boson energies, above and below \( \omega_{0,c} \).

In the former case, the TLL-CDW transition causes significant changes in the functional form of \( n(k) \). For \( \lambda > \lambda_c \), one expects an essential power law singularity at \( k_F \), corresponding to a vanishing quasiparticle weight. For finite TLL systems the difference \( \Delta = n(k_F - \delta) - n(k_F + \delta) \) is finite (with \( \delta = \pi/66 \) in our case)\(^16\). \( \Delta \) rapidly decreases approaching the CDW transition point with decreasing \( \lambda \) (see data for \( \omega_0 = 2 \) (red squares)). In the CDW phase the singularity at \( k_F \) vanishes. Note that the periodicity of \( n(k) \) doubles at \( \lambda = 0 \), in accordance with a \( R(6) \) NN-only hopping channel. To substantiate this reasoning we have included in Fig. 4 \( n(k) \)-data calculated for the 1D Hubbard model with additional NNN-transfer \( t' \). We see that \( n(k) \) of the fermion-boson model \(^11\) is in qualitative agreement with our data and previous results for the \( t \)-\( t' \) Hubbard model\(^15\), in particular for the case \( t = 0 \). The upturn in \( n(k) \) for \( k > k_F \) persists even in the metallic regime as long as NN hopping processes triggered by the (CDW) correlations in the background are of importance.

For \( \omega_0 = 1 \) the system stays metallic for all \( \lambda \). Besides the usual renormalization of \( n(k) \) with increasing correlations (i.e. decreasing \( \lambda \)) we find a slight upturn in \( n(k) \) for \( k \lesssim k_F \). This might be attributed to the fact that in our model \(^11\) a particle injected with \( k = \pm \pi \) is almost unaffected by bosonic fluctuations (which holds also for the single-particle case\(^9\)). So to speak the system behaves as a nearly perfect metal at this point. It is worth to mention that an increase in \( n(k) \) for both \( k \lesssim k_F \) and \( k \gtrsim k_F \) has been found also for the momentum distribution function of the Hubbard model (with and without magnetization) using the Gutzwiller variational wave function\(^18\).

### C. Optical response

Finally we consider the evolution of the optical conductivity going from the correlated TLL to the CDW phase at \( \omega_0 = 2 \). The corresponding optical absorption spectra
are depicted in Fig. 5. In the metallic state most of the spectral weight resides in the coherent Drude part. At $\lambda = 1$ (see inset), we find $\pi D/N \simeq 1.6$, which has to be compared with $S_{\text{reg}}(\infty) \simeq 0.2$ (of course $D$ decreases as $\lambda$ gets smaller). In this case the wave-vector resolved single-particle spectra roughly extends from $\omega = -6$ to $\omega = 6$. The regular part of the conductivity is mainly due to excitations to the phononic side bands appearing in the sectors with momenta far away from $k_F$. In the insulating region (see main panel), the first peak at about $\omega \approx 0.5$ can be assigned to an optical excitation across the gap in the (coherent) two-band structure. These excitations are only accessible for $\lambda > 0$. Additional excitations with higher energy occur around multiples of the boson frequency, where $\omega \simeq \omega_0 = 2$ sets a absorption threshold for the $\lambda = 0$ case. As expected for an insulating system with OBC, the whole spectral weight is contained in $S_{\text{reg}}(\infty) \simeq -\pi E_{\text{kin}}/2$. We emphasize that the CDW state in our model contains less than one boson per site on average, unlike e.g. the Peierls insulating state in the Holstein model. That is the CDW phase typifies rather as a correlated insulator—such as the Mott-Hubbard insulator—and no divergence occurs at the optical absorption threshold.

IV. SUMMARY

In conclusion, we have determined the spectral properties of a highly non-trivial two-channel fermion-boson transport model for the 1D half-filled band case, using an unbiased DDMRG technique. The background medium, parameterized by bosonic degrees of freedom, strongly influences the charge carrier dynamics, as it happens in many novel materials. If the background fluctuations dominate we find diffusive transport. In opposite case of strong background correlations coherent quantum transport may evolve on a reduced energy scale. These correlations can also trigger a metal insulator transition. The insulating CDW state has an asymmetric band structure, leading to characteristic signatures in the ARPES and optical response. Whether an extended model with spinful fermions gives rise to an attractive metallic phase like in the Holstein-Hubbard model would be an interesting question for further research.

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