Correlation-Induced Metal Insulator Transition in a Two-Channel Fermion-Boson Model

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We investigate charge transport within some background medium by means of an effective lattice model with a novel form of fermion-boson coupling. The bosons describe fluctuations of a correlated background. By analyzing ground state and spectral properties of this transport model, we show how a metal-insulator quantum phase transition can occur for the half-filled band case. We discuss the evolution of a mass-asymmetric band structure in the insulating phase and establish connections to the Mott and Peierls transition scenarios.

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The way a material evolves from a metallic to an insulating state is one of the most fundamental problems in solid state physics. Besides band structure and disorder effects, electron-electron and electron-phonon interactions are the driving forces behind metal-insulator transitions (MITs) in the majority of cases. While the so-called Mott-Hubbard MIT [1] is caused by strong Coulomb correlations, the Peierls MIT [2] is triggered by the coupling to vibrational excitations of the crystal. Both scenarios are known to compete in subtle ways.

The MIT problem can be addressed by the investigation of generic Hamiltonians for interacting electrons and phonons like the Holstein [3,4], Hubbard [1] and (quarter-filled) *t*-*J* models [5], or combinations of these [6]. These models have been proved to describe MIT phenomena for the half-filled band case, in particular, for one-dimensional (1D) systems known to be susceptible to the formation of insulating spin-density-wave (SDW) or charge-density-wave (CDW) broken-symmetry ground states [7]. On the metallic side of the MIT, charge transport then takes place within a "background medium" that exhibits strong correlations, which anticipate the SDW or CDW on the insulating side. In that case, a particle, as it moves, creates local distortions of substantial energy in the background. These distortions may be parametrized as bosons. They are able to relax, with a rate that depends on the system properties but also on the proximity to the MIT.

In order to model such a situation the authors recently proposed a simplified transport Hamiltonian [8,9]

$$H = H_b - \lambda\sum_i (b_i^\dagger + b_i) + \omega_0 \sum_i b_i^\dagger b_i, \qquad (1)$$

where $H_b = -t_b \sum_{\langle i,j\rangle} c_j^\dagger c_i (b_i^\dagger + b_j)$ describes the boson-affected nearest-neighbor (NN) hopping of fermionic particles ($c_i^\dagger$) [10]. In (1) the particle creates a boson ($b_i^\dagger$) on the site it leaves and destroys a boson on the site it enters. Thereby it generates a "string" of local bosonic fluctuations with energy ω_0 [11]. Cutting the string, the λ term allows a boson to decay spontaneously. A unitary transformation $b_i \mapsto b_i + \lambda/\omega_0$ eliminates the boson relaxation term in favor of a free-particle hopping channel, $H_f = -t_f \sum_{\langle i,j\rangle} c_j^\dagger c_i$ with $t_f = 2\lambda t_b/\omega_0$, in addition to the original one. As a result

$$H \mapsto H = H_b + H_f + \omega_0 \sum_i b_i^\dagger b_i, \qquad (2)$$

and the physics of our model is governed by two parameter ratios: the relative strengths of the two transport channels (t_f/t_b) and the rate of bosonic fluctuations $(\omega_0/t_b)^{-1}$. The model has been solved numerically in the one-particle sector and revealed—despite its seeming simplicity—a surprisingly rich "phase diagram" with regimes of quasi-free, correlation and fluctuation dominated transport [9]. In this case the spinless Hamiltonian (2) covers basic features of the more complicated *t*-*J*, Hubbard or Holstein models in the low doping or density regimes, but is much easier to evaluate.

Whether our two-channel transport model likewise describes a quantum phase transition from a metallic to an insulating phase at certain commensurate band fillings remained an important but open question. The free hopping channel H_f will clearly act against any correlation-induced charge ordering that might open a gap at the Fermi energy E_F. Strong bosonic fluctuations, i.e., small ω_0, will also tend to destroy CDW order. On the other hand, a tendency towards CDW formation at half-filling is expected for large ω_0/t_b by perturbative arguments, yielding an effective Hamiltonian with nearest-neighbor fermion repulsion. In some respects this is evocative of the quantum phase transition in the spinless fermion Holstein model, which for large phonon frequencies and strong couplings can be mapped on the *XXZ* model [4]. The *XXZ* model undergoes a Kosterlitz-Thouless transition at the spin isotropy point.

Further evidence of a quantum phase transition comes from the investigation of simplified versions of (1): (i) a coarse-grained model with only one bosonic oscillator for the 1D infinite system, and (ii) a 1D model based on a 2-site cluster. The exact solution of (i) and an approximate solution of (ii) both exhibit quantum phase transitions at $\lambda = 0$ between two Fermi liquids, with different Fermi surfaces, non-Fermi-liquid behavior persisting down to zero temperature at the critical point in case (ii) [8].

The MIT is a subtle quantum mechanical problem, however, that requires nonapproximative investigation schemes. Therefore, in this work, we apply unbiased numerical techniques to study the competition between itinerancy, correlations and fluctuations for the 1D half-filled band case, using the full model (1) without any restrictions. To this end we employ exact diagonalization in combination with kernel polynomial expansion methods, adapted for coupled fermion-boson systems [12]. The computational requirements are determined by the Hilbert space dimension $D_H = (N + N_b)!/[(N - N_e)!N_e!N_b!]$, where N is the number of lattice sites, N_e counts the fermions, and N_b is the maximum number of bosons retained. Typically we deal with D_H of about 10^{11}.

Let us start with the discussion of the photoemission (PE) spectra. The spectral density of single-particle excitations associated with the injection of an electron with wave vector k, $A^+(k, \omega)$ (inverse PE), and the corresponding quantity for the emission of an electron, $A^-(k, \omega)$ (PE), are given by $A^\pm(k, \omega) = \sum_n |\langle \psi_n^\pm | c_k^\pm | \psi_0 \rangle|^2 \delta[\omega \mp \omega_n^\pm]$. Here $c_k^+ = c_k^\dagger$, $c_k^- = c_k$, and $|\psi_0\rangle$ is the ground state in the N_e-particle sector while $|\psi_n^\pm\rangle$ denote the nth excited states in the $N_e \pm 1$-particle sectors with excitation energies $\omega_n^\pm = E_n^\pm - E_0$.

Figure 1 displays the wave vector resolved single-particle spectra in the regime where distortions of the background are energy intensive; i.e., the boson frequency ω_0 is high. If the free transport channel is dominant ($t_f = 5$—upper graph), the occupied (unoccupied) band states, probed by PE (inverse PE), give rise to an almost particle-hole symmetric absorption spectrum $A_K^+(\omega - E_F) \simeq A_{K-\pi}^-(E_F - \omega)$. Thereby the main spectral weight resides in the uppermost (lowest) peaks of A_K^- (A_K^+) in each K sector. The corresponding "coherent" band structure roughly follows the $-2t_f \cos K$ tight-binding band. Satellites with less spectral weight occur near the Brillouin zone boundary predominantly, as a result of mixed electron-boson excitations with total wave vector K. At $T = 0$ the Fermi energy is obtained from $\sum_K \int_{-\infty}^{E_F} A_K(\omega) d\omega = N_e = N/2$ (half-filling, no spin). We see that there is no gap between $A_{\pm\pi/2}^+$ and $A_{\pm\pi/2}^-$ at E_F. Moreover the spectral weight of both peaks is almost one; i.e., a particle injected (removed) with $K = K_F = \pm\pi/2$ propagates unaffected by bosonic fluctuations. The system behaves as an unusual metal.

If we decrease λ (t_f/t_b ratio) at fixed ω_0, we enter the regime where boson-assisted transport becomes important (see lower graph of Fig. 1). At about $\lambda_c(\omega_0 = 2) \simeq 0.1$ a gap opens at $K = \pm\pi/2$ in the PE spectra. The gap increases as $\lambda < \lambda_c$ gets smaller, but its magnitude shows no

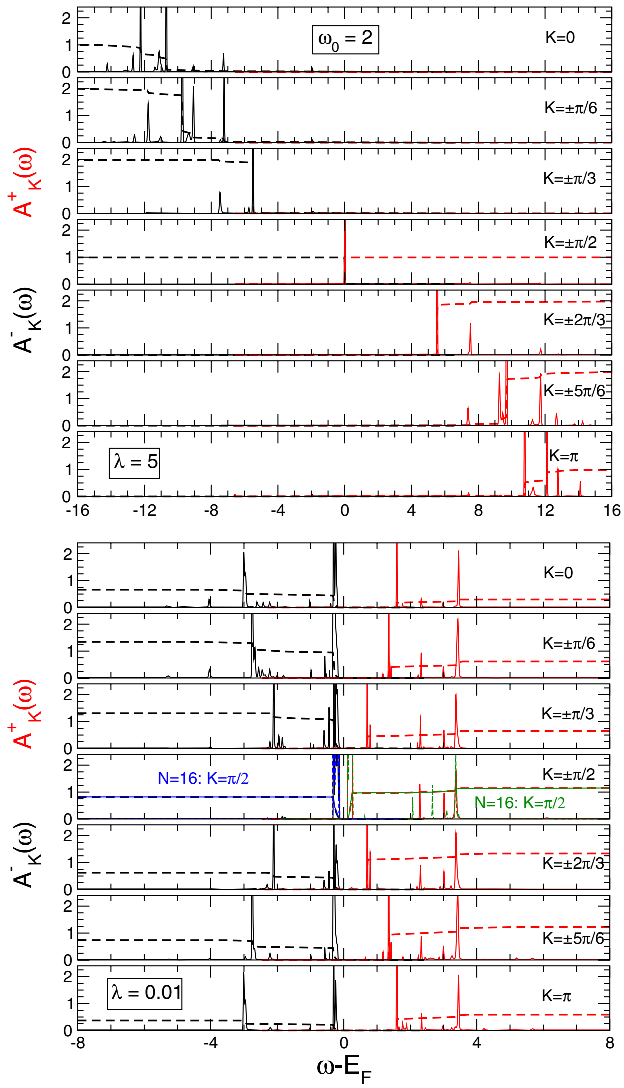

FIG. 1 (color online). Photoemission (black) and inverse photoemission spectra (red) for the half-filled band case with $\omega_0 = 2$ at $t_f = 5$ (upper panels) and $t_f = 0.01$ (lower panels), where $N = 12$, $N_b = 15$. Dashed lines give the integrated spectral weights, e.g., $S_K^+(\omega - E_F) = \int_0^\omega d\omega' A_K^+(\omega' - E_F)$, where $S_K = S_K^-(-\infty) + S_K^+(\infty) = 1$, and $\sum_K S_K = N$. Here and in what follows periodic boundary conditions were used, leading to discrete $K(N)$ wave numbers. All energies are measured in units of $t_b = 1$, and ω is rescaled with respect to E_F.

finite-size dependence (to demonstrate this we included the $N = 16$, $N_b = 9$ data for $K = \pm\pi/2$). Most notably E_F lies inside the gap region, signalizing the transition to the insulating state. The MIT is correlation induced. Since λ is small, distortions of the background cannot relax easily. Accordingly the band structure is strongly renormalized. We observe that now $A_K^\pm(\omega - E_F) \simeq A_{\pi-K}^\pm(\omega - E_F)$ and expect a perfect doubling of the Brillouin zone for $N \to \infty$. Mapping our model (1) for $\omega_0 \gg t_f$, t_b to a (XXZ-like) spin model, $S_z \to -S_z$ symmetry is broken, reflecting the observed broken particle-hole symmetry: the highest occupied states belong to an extremely flat quasiparticle

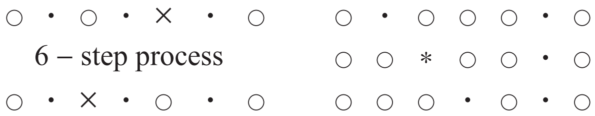

FIG. 2. Doping a perfect CDW, states with one particle removed (left panel) are connected by a six-step hopping process (see text), whereas a two-step process (right panel) relates states with an additional particle.

band, whereas the lowest unoccupied states are much more dispersive [13].

The correlated band structure can be understood by "doping" a perfect CDW state (Fig. 2). To restore the CDW order a doped hole can be transferred by a coherent 6-step process of order $\mathcal{O}(t_b^6/\omega_0^5)$,

$$|\circ\cdot\cdot\rangle \to |*\circ\cdot\rangle \to |**\circ\rangle \to \left|*\binom{*}{\circ}*\right\rangle \to |\circ **\rangle \to |\cdot\cdot\circ\rangle,$$

where in steps 1–3, three bosons ($*$) are excited, which are consumed in steps 4–6 afterwards [9,14]. In this process the fermion ($\circ$) becomes correlated with the background fluctuations. We note that such a coherent hopping process, in which the particle propagates and restores the background, exists even for the case $\lambda = 0$ where transport is fully boson-assisted. In contrast an additional electron can move by a two-step process of order $\mathcal{O}(t_b^2/\omega_0)$. Consequently, the electron band is much less renormalized than the hole band, and the mass enhancement is by a factor $\mathcal{O}((t_b/\omega_0)^4)$ smaller. Note that the mass-asymmetric band structure that evolves here is correlation induced.

That the observed MIT is indeed correlation induced is corroborated by the weakening and finally closing of the excitation gap if the boson energy ω_0 is reduced at fixed λ (see Fig. 3). In this way the ability of the background to relax is enhanced, fluctuations overcome correlations and the system turns back to a metallic state. At the same time the spectral weight is transferred from the coherent to the incoherent part of the (inverse) PE spectra, especially for K away from $K_F = \pi/2$ where the line shape is affected by rather broad bosonic signatures.

The CDW structure of the insulating state becomes apparent by investigating the particle-particle and particle-boson correlation function, $\chi_{ee}(j) = \frac{1}{N_e^2}\sum_i \langle n_i n_{i+j}\rangle$ and $\chi_{eb}(j) = \frac{1}{N_e}\sum_i \langle n_i b_{i+j}^\dagger b_{i+j}\rangle$, respectively, where $n_i = c_i^\dagger c_i$.

In Fig. 4 the even-odd modulation of the charge density away from a singled out site i of the first particle is clearly visible. We note that the charge structure factor, $S_c(\pi) = \frac{1}{N^2}\sum_{i,j}(-1)^j \langle 0|(n_i - 1/2)(n_j - 1/2)|0\rangle$, increases by a factor of about two in going from $\lambda = 0.1$ ($S_c = 0.0561$) to $\lambda = 0.01$ ($S_c = 0.1056$) at $\omega_0 = 2$ [15].

In the CDW, where, e.g., the even sites are occupied, every hop of a fermion excites a boson at an even site. This gives a large contribution to $\chi_{eb}(j)$ at even sites in addition to NN sites $|j| = 1$ (middle panel). Since the CDW involves only few bosons (see lower panel), this is the

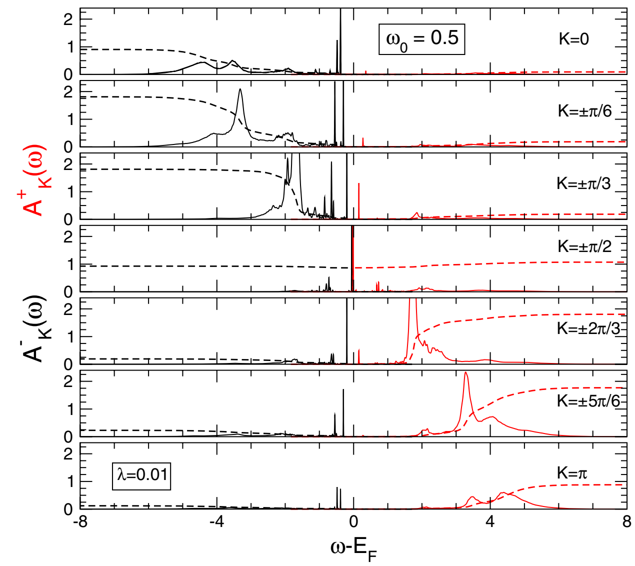

FIG. 3 (color online). (Inverse) Photoemission for $\omega_0 = 0.5$ and $\lambda = 0.01$, i.e., $t_f(\lambda, \omega_0) = 0.04$. Again $N = 12$, but now $N_b = 15$.

dominant contribution in first order of t_b/ω_0, and explains why the boson density is large at sites with large fermion density, although the hopping term t_b creates bosons at the neighboring sites of a fermion.

The charge oscillations become rapidly suppressed by increasing λ, but there is still a reduced charge density at the particle's neighboring sites, which enhances the mobility of the carrier. Accordingly the boson density is enlarged (suppressed) at the NN sites (site) of the particle. Clearly, $\chi_{eb}(j)$ is small $\forall\, |j|$ if $\omega_0 \gg t_b, t_f$ because of the high energy cost. As expected, the fluctuation dominated

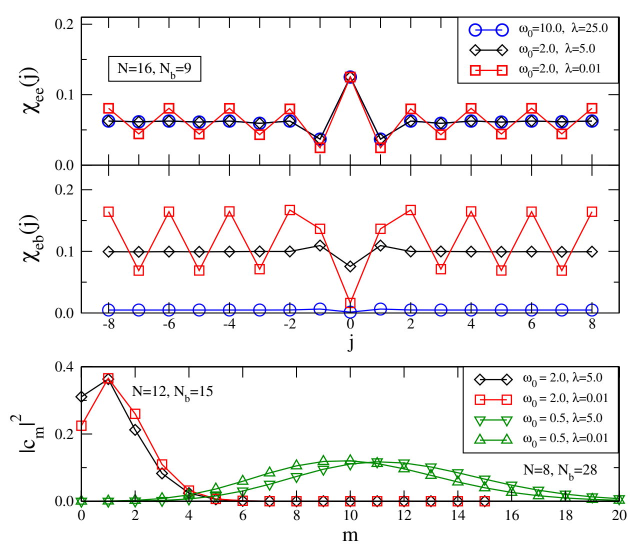

FIG. 4 (color online). Particle-particle (χ_{ee}), respectively, particle-boson (χ_{eb}) correlation functions [upper graph], and weight of the m-boson state ($|c_m|^2$) [lower panel] in the ground state of the half-filled 1D two-channel fermion-boson model (2).

regime is characterized by a large number of boson quanta in the ground state. The position of the maximum in the boson weight function $|c_m|^2$ is shifted to slightly larger values as λ increases; i.e., the correlations weaken.

Further information on the ground state properties can be obtained from the kinetic energy parts $E_{\mathrm{kin},f/b} = \langle 0|H_{f/b}|0\rangle$. By way of example, at $\omega_0 = 2$ ($N = 12$, $N_b = 15$), we find $E_{\mathrm{kin},f} = -37.040$ $[-0.023]$ and $E_{\mathrm{kin},b} = -5.291$ $[-7.125]$ for $\lambda = 5.0$ $[0.01]$, showing that boson-assisted hopping becomes the major transport mechanism at small λ. On the metallic side of the MIT the creation and annihilation of bosons opens a coherent transport channel in the regime where strong correlations persist in the background. The Drude weight D, obtained from the f-sum rule $-D = \frac{1}{2}(E_{\mathrm{kin},f} + E_{\mathrm{kin},b}) + \int_0^\infty \sigma_{\mathrm{reg}}(\omega)d\omega$, serves as a measure for this coherent transport. Here $\sigma_{\mathrm{reg}}(\omega) = \sum_{n>0} \frac{|\langle n|j|0\rangle|^2}{\omega_n} \delta(\omega - \omega_n)$ is the regular part of the optical conductivity (with current $j = j_f + j_b$). D is reduced with decreasing λ; e.g., we have $D = 20.29$ [5.146] for $\lambda = 5.0$ [1.0] at $\omega_0 = 2$.

At the MIT point D vanishes for the infinite system. At the same time the optical gap opens. In the insulating phase the optical response is dominated by the multiboson emission and absorption processes. Thus the spectral weight contained in the regular part of $\sigma(\omega)$ is enhanced.

A small boson frequency allows for large fluctuations in the background, i.e., many bosons in our model. This supports transport via the 6-step process on the one hand but, as in the one-particle sector [9], also limits the mobility of a particle by many scattering events. Nevertheless D is expected to stay finite even for $\omega_0/t_b \rightarrow 0$.

To summarize, the two-channel transport Hamiltonian, introduced for studying the dynamics of charge carriers in a correlated/fluctuating medium, has previously only been properly analyzed for a single carrier [9]. In this limit the model may capture some of the physics of 2D high-T_c superconducting cuprates [16] or 3D colossal magnetoresistive manganites [17]. Here we focused on the metal-insulator transition problem at finite particle density, in particular, in one dimension at half-filling, which might be of importance, e.g., for the 1D CDW MX chain compounds [7]. Since in this case the problem is of the same complexity as for the quarter-filled t-J_z-$J_\perp$ or spinless fermion Holstein models, we make use of elaborate numerical techniques in order to avoid uncontrolled approximations. From our finite-cluster study we have strong evidence that the model exhibits a quantum phase transition from a metallic to an insulating state. The MIT is driven by correlations, like the Mott-Hubbard transition, but in our case true long-range order develops because a CDW state is formed. This might point towards a Peierls transition scenario. The Peierls instability, however, is most pronounced in the adiabatic limit of small phonon frequencies, with many phonons involved in establishing the CDW (lattice dimerization). By contrast, we find that the CDW ground state is a few-boson state. Obviously, the system is more susceptible to CDW-formation at large boson frequency ω_0 (small transfer amplitude t_f), keeping the boson relaxation $\lambda = t_f\omega_0/2t_b$ fixed. This is the limit of an effective fermionic system with (instantaneous) Coulomb repulsion. Recall that as a consequence of the correlation-induced CDW state, a band structure with a very narrow valence and broad conduction band evolves, different in nature from simple two-band models.

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