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Metal-insulator transition in the Edwards model

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Abstract. To understand how charge transport is affected by a background medium and vice versa we study a two-channel transport model which captures this interplay via a novel, effective fermion-boson coupling. By means of (dynamical) DMRG we prove that this model exhibits a metal-insulator transition at half-filling, where the metal typifies a repulsive Luttinger liquid and the insulator constitutes a charge density wave. The quantum phase transition point is determined consistently from the calculated photoemission spectra, the scaling of the Luttinger liquid exponent, the charge excitation gap, and the entanglement entropy.

The way a system evolves from a metallic to an insulating state is one of the most fundamental problems in solid state theory. Electron-electron and electron-phonon interactions are the driving forces behind metal-insulator transitions (MITs) in the majority of cases. For example, the Mott-Hubbard MIT [1] is caused by strong Coulomb correlations, whereas the Peierls MIT [2] is triggered by the coupling to vibrational excitations of the crystal. Theoretically the MIT problem can be addressed by the investigation of generic Hamiltonians for interacting electrons and phonons such as Hubbard or Holstein models [3]. In one dimension (1D), these models exhibit a MIT at half-filling, where on the insulating side of the MIT a spin-density-wave (SDW) or a charge-density-wave (CDW) broken-symmetry ground state appears, respectively. On the metallic side, near the MIT, charge transport then takes place within a strongly correlated "background" that anticipates the developing SDW, respectively CDW, order. Since the particles responsible for charge transport and the background order phenomena are the same, the problem is very complex.

A path forward might be the construction of simplified transport models, which capture the basic mechanisms of quantum transport in a background medium in a rather effective way. Along this line a novel quantum transport model has been proposed recently [4],

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

This so-called Edwards model mimics the correlations inherent to a spinfull fermionic many-particle systems by a boson affected hopping of spinless particles (see Fig. 1). For the half-filled band case, the model describes a repulsive Tomonaga-Luttinger liquid (TLL), provided the excitations of the background are energetically inexpensive ($\omega_0 < \omega_{0,c}$) or will readily relax ($\lambda > \lambda_c(\omega_0)$). This defines the fluctuation dominated regime. By contrast, strong background correlations, which will develop for large ω_0 and small $\lambda \ll t_b$ tend to immobilize the charge carriers and may even drive a MIT by establishing CDW long-range order [5].

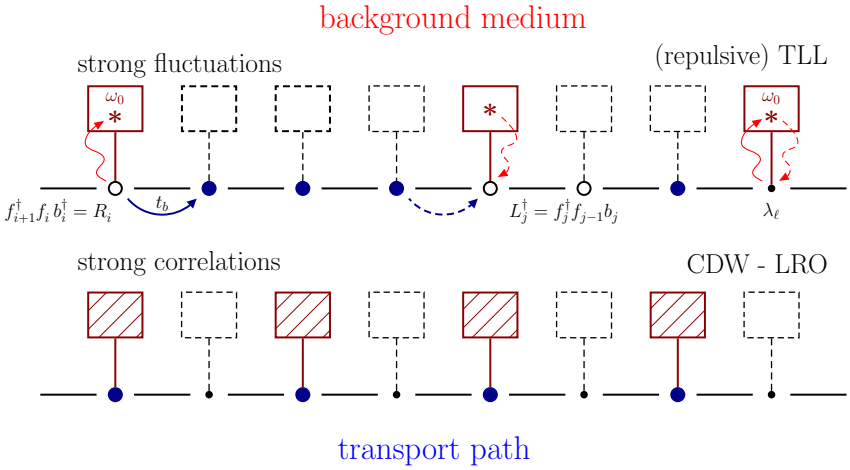

Figure 1. The Edwards model (1) describes a very general situation: As a charge carrier (•) moves along a 1D transport path it creates an excitation with energy ω_0 ($*$) in the background at the site it leaves or annihilates an existing excitation at the site it enters. The background medium may represent, e.g., a magnetically, orbitally or charge ordered lattice. One assumes that the (de)excitation of the background can be parameterized as a bosonic degree of freedom. Any distortion of the background can heal by quantum fluctuations. Accordingly the λ-term allows for spontaneous boson creation and annihilation processes.

In the present work, we employ density-matrix renormalization group (DMRG) and dynamical DMRG methods [6] to analyse the ground-state properties of the Edwards model and the charge carrier dynamics for the limiting case of high-energy background fluctuations.

Let us start with the discussion of the photoemission (PE) spectra. The single-particle spectral function probed by angle-resolved [inverse] PE reads

$$A(k,\omega) = A^-(k,\omega) + A^+(k,\omega)\,, \quad \text{with} \quad A^\pm(k,\omega) = \sum_n |\langle\psi_n^\pm|f_k^\pm|\psi_0\rangle|^2\,\delta[\omega \mp \omega^\pm]\,. \tag{2}$$

Here $A^-(k,\omega)$ $[A^+(k,\omega)]$ is associated with the emission [injection] of an electron with wave vector k, i.e. $f_k^- = f_k$ and $f_k^+ = f_k^\dagger$. $|\psi_0\rangle$ is the ground state of a N–site system in the N_f–particle sector, while $|\psi_n^\pm\rangle$ denote the n-th excited states in the $N_f \pm 1$-particle sectors with excitation energies $\omega_n^\pm = E_n^\pm - E_0$. For the half-filled Edwards model we have $N_f = N/2$.

Figure 2 shows $A(k,\omega)$ for a stiff background, i.e. the distortions induced by particle hopping are energetically costly. In this regime the bosons will strongly affect particle transport: The quasiparticle mass is sizeably enhanced and a renormalized band structure appears but—if λ is large enough—the system remains metallic, as can be seen from the finite spectral weight at the Fermi energy E_F (left panel). As the system's ability for relaxation decreases, i.e., at fixed ω_0, λ falls below a certain critical value, a gap opens in the single-particle spectrum at $k_F = \pi/2$ (middle panel). Evidently the system has become an insulator. We note the internal feedback mechanism: The collective boson excitations originate from the motion of the charge carriers and have to persist long enough to finally inhibit particle transport, thereby completely changing the nature of the many-particle ground state. The collective boson-particle dynamics leads to an asymmetric band structure for $k \leq k_F$ and $k \geq k_F$ (see inset). While the induced hole probed by PE can only move coherently by a six-step process with three bosons first excited and afterwards consumed, an additional electron can easily move by a two-step process even if strong CDW correlations exist in the background [5]. We note that the (I)PE spectra exhibit weak

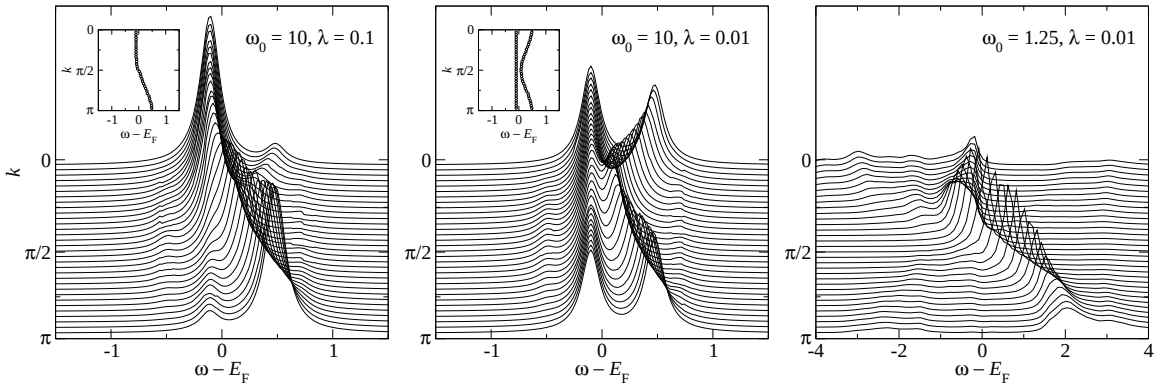

Figure 2. Line-shape of the single-particle spectral $A(k,\omega)$ in the half-filled band sector of the 1D Edwards model. The insets shows the dispersion of the absorption/emission maximum. For the numerics, we consider an $N = 32$–site chain with open boundary conditions (BC) and map a boson site, containing 2^{n_b} states, to n_b pseudosites. We take up to 4 pseudosites, keep $m = 500$ density-matrix eigenstates, and use a broadening $\eta = 0.1$. All energies are given in units of t_b.

signals around the bare boson energies $\pm\omega_0$ (not shown). The interrelation of charge dynamics and background fluctuation becomes apparent again, if we decrease ω_0 keeping λ fixed (right panel). Now the fluctuations overcome the correlations and the system returns to a metallic state which is different in nature, however, from the state we started with: $A(k,\omega)$ shows sharp absorption features near k_F only and is "overdamped" at the Brillouin zone boundaries, where the spectrum is dominated by bosonic excitations.

In order to determine more precisely the phase boundary between the metallic and insulating ground states, typifying a Tomonaga-Luttinger liquid (TLL) and a CDW, respectively, we analyse the limiting ($N \to \infty$) behaviour of the TLL charge exponent

$$K_\rho = \pi \lim_{q\to 0} \frac{S_c(q)}{q}\,, \quad \text{with} \quad S_c(q) = \tfrac{1}{N}\sum_{i,j} \mathrm{e}^{\mathrm{i}q(j-k)} \langle (n_j - \tfrac{1}{2})(n_k - \tfrac{1}{2})\rangle\,, \;\; q = \frac{2\pi}{N}, \tag{3}$$

as well as those of the single-particle (charge) gap, $\Delta_c(N) = E_0^+ + E_0^- - 2E_0$, and monitor the finite-size scaling of the entanglement entropy difference [7]

$$\Delta S_N = S_N(N/2) - S_N(N/2-1) = -\frac{c^*}{3} \ln\cos\left[\frac{\pi}{N}\right]\,, \tag{4}$$

where $S_N(l) = -\mathrm{Tr}[\rho_l \ln \rho_l] = \frac{c^*}{3} \ln\left[\frac{N}{\pi}\sin\left(\frac{\pi l}{N}\right)\right] + s_1$. We expect that the TLL charge exponent decreases from $K_\rho = 1$, as λ is lowered, and finally reaches $1/2$ at the MIT point, if the transition is of Kosterlitz-Thouless type [8, 9]. The central charge c^* should scale to unity in the metallic TLL regime [10].

Figure 3 demonstrates that the $N \to \infty$ extrapolated K_ρ indeed becomes $1/2$ at some critical value, where $\lambda_c^{-1}(\omega_0 = 10) \simeq 5.89$, indicating the MIT. In the metallic phase we find a repulsive particle interaction, $K_\rho \leq 1$. Our DMRG results point towards an exponential opening of the charge gap entering the insulating state, which corroborates the Kosterlitz-Thouless transition scenario. Note that the CDW state of the Edwards model is a few boson state, in contrast to the Peierls CDW phase of the Holstein model [5]. That means the MIT in the Edwards model is driven by strong correlations, as for the Mott-Hubbard transition. To extract the central charge c^* we use the entanglement entropy difference, Eq. (4), rather than directly exploiting $S_N(l)$.

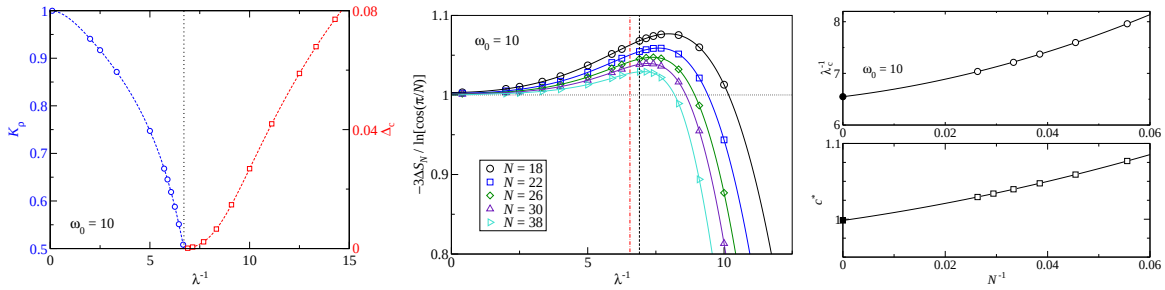

Figure 3. Left panel: $N \to \infty$ extrapolated value of the TLL parameter K_ρ, respectively of the charge gap Δ_c, as a function of λ^{-1} for $\omega_0 = 10$ (open BC). Middle panel: Entanglement entropy differences ΔS_N for different system sizes (periodic BC). The red dashed-dotted line gives the MIT transition point in reasonable agreement with the value obtained from K_ρ (black dashed line). Right panels: Critical value of λ_c^{-1} (filled circle, top panel) and central charge $c^* \simeq 1$ (filled square, bottom panel), both extrapolated from the maxima of ΔS_N. Here we use $m = 2000$, $n_b = 2$, and ensure a discarded weight less than 10^{-10}.

For a model with spinless fermions this is advantageous because we can work with a fixed system size, thereby avoiding antiperiodic BC that give rise to complex phase factors [7]. As can be seen from the middle panel of Fig. 3, for $\lambda^{-1} < \lambda_c^{-1}$, the rescaled quantity $-3\Delta S_N / \ln[\cos(\pi/N)]$ extrapolates to unity as $N \to \infty$. This opens an alternative route to detect the MIT point. We find that the $\lambda_c^{-1}(\omega_0)$ determined by extrapolating the maximum of ΔS_N, i.e. in a completely different manner, matches the critical value obtained from K_ρ surprisingly well. Simultaneously, indeed $c^* \to 1$ (see right panel).

To summarise, we have studied the spectral and ground-state properties of the 1D Edwards fermion-boson transport model by large-scale (dynamical) DMRG numerics. We showed that strong correlations within the background medium will not only affect the charge-carrier's dynamics by enhancing the quasiparticle mass but may even trigger a metal-insulator quantum phase transition. The MIT transition point has been determined in good agreement both from the TLL charge exponent and the entanglement entropy difference. We stress that to date only a very small number of microscopic model exists which have been rigorously shown to exhibit a MIT.

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