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Charge-density-wave formation in the Edwards fermion-boson model at one-third band filling

Satoshi Ejima* and Holger Fehske†

Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, 17489 Greifswald, Germany

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We examine the ground-state properties of the one-dimensional Edwards spinless fermion transport model by means of large-scale density-matrix renormalization-group calculations. Determining the single-particle gap and the Tomonaga-Luttinger liquid parameter (K_ρ) at zero temperature, we prove the existence of a metal-to-insulator quantum phase transition at one-third band filling. The insulator—established by strong correlation in the background medium—typifies a charge density wave (CDW) that is commensurate with the band filling. $K_\rho = 2/9$ is very small at the quantum critical point, and becomes $K_\rho^{\rm CDW} = 1/9$ in the infinitesimally doped three-period CDW, as predicted by the bosonization approach.

KEYWORDS: Edwards model, metal-insulator transition, DMRG

1. Introduction

Strong correlations can affect the transport properties of low-dimensional systems to the point of insulating behavior. Prominent examples are broken symmetry states of quasi one-dimensional (1D) metals, where charge- or spin-density waves brought about by electron-phonon or by electron-electron interactions [1]. These interactions can be parametrized by bosonic degrees of freedom, with the result that the fermionic charge carrier becomes "dressed" by a boson cloud that lives in the particle's immediate vicinity and takes an active part in its transport [2]. A paradigmatic model describing quantum transport in such a "background medium" is the Edwards fermion-boson model [3, 4]. The model exhibits a surprisingly rich phase diagram including metallic repulsive and attractive Tomonaga-Luttinger-liquid (TLL) phases, insulating charge-density-wave (CDW) states [5–8], and even regions where phase separation appears [9].

The part of the Edwards Hamiltonian that accommodates boson-affected transport is

$$H_{fb} = -t_b \sum_{\langle i,j \rangle} f_j^\dagger f_i \, (b_i^\dagger + b_j) \,. \tag{1}$$

Every time a spinless fermion hops between nearest-neighbor lattice sites i and j it creates (or absorbs) a local boson $b_j^\dagger$ (b_i). As to $H_b = \omega_0 \sum_i b_i^\dagger b_i$ this enhances (lowers) the energy of the background by ω_0. Moving in one direction only, the fermion creates a string of local bosonic excitations that will finally immobilize the particle (just as for a hole in a classical Néel background). Because of quantum fluctuations any distortion in the background should be able to relax however. Incorporating this effect the entire Edwards model takes the form

$$H = H_{fb} - \lambda \sum_i (b_i^\dagger + b_i) + H_b \,, \tag{2}$$

*E-mail address: ejima@physik.uni-greifswald.de
†E-mail address: fehske@physik.uni-greifswald.de

where λ is the relaxation rate. The unitary transformation $b_i \to b_i + \lambda/\omega_0$ replaces the second term in (2) by a direct, i.e., boson-unaffected, fermionic hopping term $H_f = -t_f \sum_{\langle i,j \rangle} f_j^\dagger f_i$. In this way the particle can move freely, but with a renormalized transfer amplitude $t_f = 2\lambda t_b/\omega_0$. We note 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 being related to an effective next-nearest-neighbor transfer. This process takes place on a strongly reduced energy scale (with weight $\propto t_b^6/\omega_0^5$), and is particularly important in the extreme low-density regime ($n^f \ll 1$), where the Edwards model mimics the motion of a single hole in a quantum antiferromagnet [10].

At low-to-intermediate particle densities $n^f \leq 0.3$ the 1D Edwards model system stays metallic. If here the fermions couple to slow (low-energy) bosons ($\omega_0/t_b \lesssim 1$), the primarily repulsive TLL becomes attractive, and eventually even phase segregation into particle-enriched and particle-depleted regions takes place at small λ [9]. No such particle attraction is observed, however, for densities $0.3 \lesssim n^f \leq 0.5$. Perhaps, in this regime, the repulsive TLL might give way to an insulating state with charge order if the background is "stiff", i.e., for small λ/t_b and fast (high-energy) bosons $\omega_0/t_b > 1$. So far, a correlation induced TLL-CDW metal-insulator transition like that has been proven to exist for the half-filled band case ($n^f = 0.5$) [5, 6]. In the limit $\omega_0/t_b \gg 1 \gg \lambda/t_b$ the Edwards model can be approximated by an effective t-V model, $H_{tV} = H_f + V \sum_i n_i^f n_{i+1}^f$, with nearest-neighbor Coulomb interaction $V = t_b^2/\omega_0$ [11]. The spinless fermion t-V model on his part can be mapped onto the exactly solvable XXZ-Heisenberg model, which exhibits a Kosterlitz-Thouless [12] (TLL-CDW) quantum phase transition at $(V/t_f)_c = 2$, i.e., at $(\lambda/t_b)_{tV,c} = 0.25$. The critical value is in reasonable agreement with that obtained for the half-filled Edwards model in the limit $\omega_0 \to \infty$: $(\lambda/t_b)_c \simeq 0.16$ [6]. At lower densities, however, for example at $n^f = 1/3$, a CDW instability occurs in 1D t-V-type models only if (substantially large) longer-ranged Coulomb interactions were included, such as a next-nearest-neighbor term V_2 [13].

In order to clarify whether the 1D Edwards model by itself shows a metal-to-insulator transition off half-filling at large ω_0 and what is the reason for the absence of phase separation for small ω_0, in this work, we investigate the model at one-third band filling, using the density matrix renormalization group (DMRG) technique [14] combined with the pseudo-site approach [15, 16] and a finite-size analysis. This allows us to determine the ground-state phase diagram of the 1D Edwards model in the complete parameter range.

2. Theoretical approach

To identify the quantum phase transition between the metallic TLL and insulating CDW phases we inspect—by means of DMRG—the behavior of the local fermion/boson densities $n_i^{f/b}$, of the single-particle gap Δ_c, and of the the TLL parameter K_ρ. In doing so, we take into account up to four pseudo-sites, and ensure that the local boson density of the last pseudo-site is always less than 10^{-7} for all real lattice sites i. We furthermore keep up to $m = 1200$ density-matrix eigenstates in the renormalization process to guarantee a discarded weight smaller than 10^{-8}.

For a finite system with L sites the single-particle charge gap is given by

$$\Delta_c(L) = E(N+1) + E(N-1) - 2E(N), \tag{3}$$

where $E(N)$ and $E(N \pm 1)$ are the ground-state energies in the N- and $(N \pm 1)$-particle sectors, respectively. In the CDW state Δ_c is finite, but will decrease exponentially across the MI transition point if the transition is of Kosterlitz-Thouless type as for the t-V model. This hampers an accurate determination of the TLL-CDW transition line.

In this respect the TLL parameter K_ρ is more promising. Here bosonization field theory predicts how K_ρ should behave at a quantum critical point. In order to determine K_ρ accurately by DMRG,

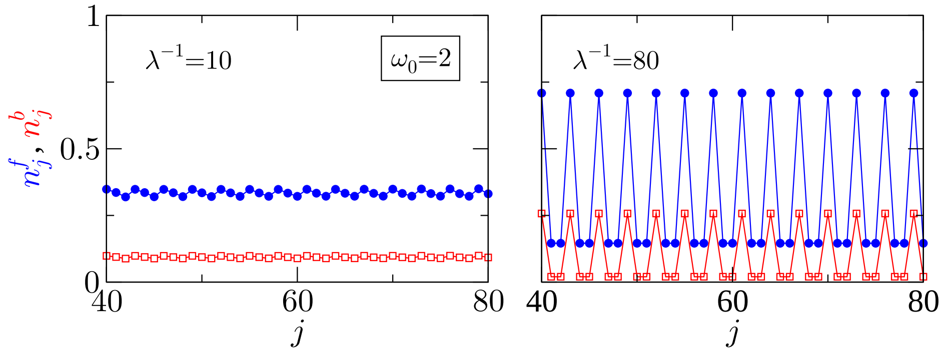

Fig. 1. (Color online) Local fermion (n_j^f – filled blue circles) and boson (n_j^b – open red squares) densities in the central part of an Edwards model chain with $L = 120$ sites and OBC. DMRG data shown in the left-hand (right-hand) panel indicate a homogeneous TLL (CDW) state for $n^f = 1/3$ and $\lambda^{-1} = 10$ ($\lambda^{-1} = 80$), where $\omega_0 = 2$. In what follows all energies are measured in units of t_b.

we first have to calculate the static (charge) structure factor

$$S_c(q) = \frac{1}{L}\sum_{j,l} e^{\mathrm{i}q(j-l)}\langle(f_j^\dagger f_j - n)(f_l^\dagger f_l - n)\rangle\,, \tag{4}$$

where the momenta $q = 2\pi m/L$ with integers $0 < m < L$ [17]. The TLL parameter K_ρ is proportional to the slope of $S_c(q)$ in the long-wavelength limit $q \to 0^+$:

$$K_\rho = \pi \lim_{q\to 0}\frac{S_c(q)}{q}\,. \tag{5}$$

For a spinless-fermion system with one-third band filling, the TLL parameter should be $K_\rho^* = 2/9$ at the metal-insulator transition point. For an infinitesimally doped three-period CDW insulator, on the other hand, bosonization theory yields $K_\rho^{\mathrm{CDW}} = 1/9$ [18, 19].

3. Numerical results

First evidence for the formation of a CDW state in the one-third filled Edwards model comes from the spatial variation of the local densities of fermions $n_i^f \equiv \langle f_i^\dagger f_i\rangle$ and bosons $n_i^b \equiv \langle b_i^\dagger b_i\rangle$. Fixing $\omega_0 = 2$, we find a modulation of the particle density commensurate with the band filling factor 1/3 for very small $\lambda = 0.0125$ (see Fig. 1, right panel). Thereby, working with open boundary conditions (OBC), one of the three degenerate ground states with charge pattern (... 100100100 ...), (... 010010010 ...), or (... 001001001 ...) is picked up by initializing the DMRG algorithm. As a result the CDW becomes visible in the local density. Note that also in the metallic state, which is realized already for λ's as small as 0.1 (cf. Fig. 1, left panel), a charge modulation is observed. Those, however, can be attributed to Friedel oscillations, which are caused by the OBC and will decay algebraically in the central part of the chain as L increases. Thus, for $\omega_0 = 2$, a metal-to-insulator transition is expected to occur in between $10 < \lambda^{-1} < 80$.

To localize the point where—at given ω_0 and λ—the quantum phase transition takes place, we first compute the single-particle gap Δ_c and TLL charge exponent K_ρ for finite chains with up to $L = 150$ sites and OBC. Then we perform a finite-size scaling as illustrated for K_ρ by Fig. 2, left panel. Here open symbols give K_ρ as a function of the inverse system size L^{-1}. The DMRG data can be extrapolated to the thermodynamic limit by third-order polynomial functions. Decreasing λ

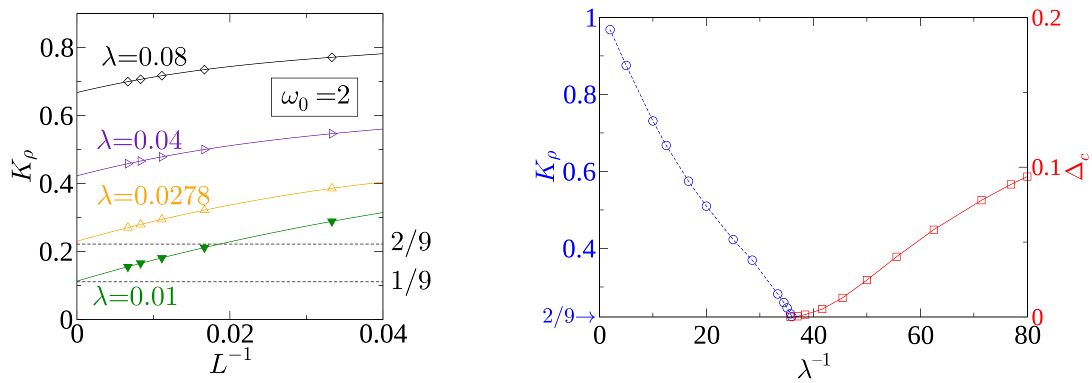

Fig. 2. (Color online) Left panel: $K_\rho(L)$ in the one-third filled Edwards model as a function of the inverse system size for various values of λ at $\omega_0 = 2$ (open symbols). The finite-size interpolated DMRG data at the metal-insulator transition point and for the infinitesimally doped CDW insulator [$n^f = 1/3 - 1/L$ (filled symbols)] are in perfect agreement with the bosonization results $K_\rho^* = 2/9$ and $K_\rho^{\rm CDW} = 1/9$, respectively. Right panel: $L \to \infty$ extrapolated K_ρ (circles) and Δ_c (squares), as functions of λ^{-1} for $\omega_0 = 2$, indicate a TLL-CDW transition at $\lambda^{-1} \sim 36$.

at fixed $\omega_0 = 2$ the values of K_ρ decreases too and becomes equal to $K_\rho^* = 2/9$ at the Kosterlitz-Thouless transition point $(\lambda^{-1})_c \sim 36$; see Fig. 2, right panel. For $\lambda^{-1} > 36$ the system embodies a $2k_{\rm F}$-CDW insulator with finite charge gap Δ_c. Furthermore, calculating $K_\rho(L)$ for $N = L/3 - 1$ particles, we can show that the infinitesimally doped CDW insulator has $K_\rho^{\rm CDW} = 1/9$ at $n^f = 1/3$. Deep in the CDW phase, K_ρ approaches $1/9$ in the thermodynamic limit [cf. the $\lambda = 0.01$ data (filled symbols) in the left panel of Fig. 2].

Our final result is the ground-state phase diagram of the one-third filled Edwards model shown in Fig. 3. The TLL-CDW phase boundary is derived from the $L \to \infty$ extrapolated K_ρ values. Within the TLL region $2/9 < K_\rho < 1$. Of course, the TLL appears at large λ, when any distortion of the background medium readily relaxes ($\propto \lambda$), or, in the opposite limit of small λ, when the rate of the bosonic fluctuations ($\propto \omega_0^{-1}$) is sufficiently high. Below $\omega_{0,c} \simeq 0.93$ the metallic state is stable $\forall\lambda$, because the background medium is easily disturbed and therefore does not hinder the particle's motion much. Note that this value is smaller than the corresponding one for the half-filled band case, where $\omega_{0,c} \simeq 1.38$. On the other hand, the $2k_{\rm F}$-CDW phase with $\Delta_c > 0$ and long-range order appears, at half-filling, for small λ and by trend large ω_0 (see dashed lines); $\lambda_c \simeq 0.16$ for $\omega_0 \to \infty$ [6]. Interestingly, for $n^f = 1/3$, we observe that the CDW will be suppressed again if the energy of a background distortion becomes larger than a certain λ-dependent value (see Fig. 3, left panel). In stark contrast to the half-filled band case, at $n^f = 1/3$, it seems that the TLL is stable $\forall\lambda$, when $\omega_0 \to \infty$. This is because in this limit in the corresponding one-third filled t-V model not only a nearest-neighbor Coulomb repulsion V but also a substantial next-nearest-neighbor interaction V_2 is needed to drive the TLL-to-CDW transition [13]. Again in the limit $\omega_0/t_b \gg 1 \gg \lambda/t_b$, the Edwards model at one-third filling can be described by the effective t-V-V_2 model with $V = 2t_b^2/3\omega_0$ and $V_2 = 2t_b^4/\omega_0^3$, i.e., $V_2/t_f = t_b^3/\lambda\omega_0^2$, which clearly explains the absence of the CDW phase for $\omega_0 \gg 1$.

4. Conclusions

To summarize, using an unbiased numerical (density matrix renormalization group) technique, we investigated the one-dimensional fermion-boson Edwards model at one-third band filling. We proved that the model displays a metal-insulator quantum phase transition induced by correlations in

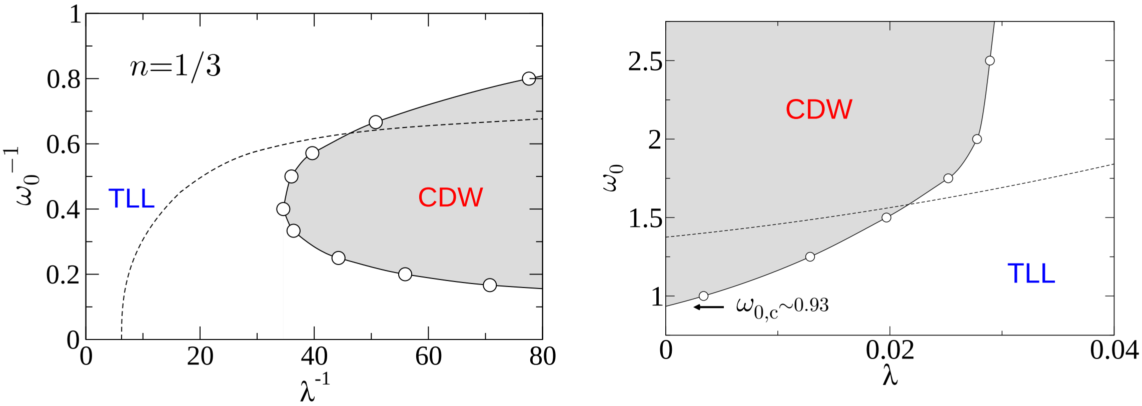

Fig. 3. (Color online) DMRG ground-state phase diagram of the 1D Edwards model at one-third band filling, showing the stability regions of metallic TLL and insulating CDW phases in the λ^{-1}-ω_0^{-1} (left panel) and λ-ω_0 (right panel) plane. The dashed line denotes the MI transition points at half band filling from Ref. [6].

the background medium. The metallic phase is a Tomonaga-Luttinger liquid with $2/9 < K_\rho < 1$. The insulator represents a $2k_{\rm F}$ charge density wave with $K_\rho^{\rm CDW} = 1/9$ deep inside the long-range ordered state. Performing a careful finite-size scaling analysis, the phase transition point can be precisely determined by K_ρ. If the background medium is stiff, we can conclude—by analogy with the ground-state phase diagram of the one-third filled t-V-V_2 model—that the Edwards model incorporates the effects of both effective nearest-neighbor and next-nearest-neighbor Coulomb interactions between the fermionic charge carriers. The effect of the latter one is reduced when the energy of a local distortion in the background is very large, which maintains metallic behavior—different from the half-filled band case—even for weak boson relaxation.

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