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

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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 ($K_\rho$) 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 $K_{\rho_{CDW}} = 1/9$ 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

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

Every time a spinless fermion hops between nearest-neighbor lattice sites $i$ and $j$ it creates (or absorbs) a local boson $b_i^\dagger (b_j)$. As to $H_b = \omega_0 \sum_i b_i^\dagger b_i$, this enhances (lowers) the energy of the background by $\omega_0$. 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

\begin{equation}
H = H_{fb} - \lambda \sum_i (b_i^\dagger + b_i) + H_b,
\end{equation}

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where $\lambda$ is the relaxation rate. The unitary transformation $b_i \rightarrow b_i + \lambda/\omega_0$ replaces the second term in (2) by a direct, i.e., boson-unaffected, fermionic hopping term $H_f = -t_f \sum_{\langle i,j \rangle} f_i \dagger f_j$. 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 $\propto t_b^6/\omega_0^3$), 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 $n_f \lesssim 0.3$ 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 $\lambda$ [9]. No such particle attraction is observed, however, for densities $0.3 \lesssim n_f \lesssim 0.5$. 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 $\lambda/t_b$ 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 $\omega_0 \rightarrow \infty$: $(\lambda/t_b)_c \simeq 0.16$ [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 $\omega_0$ and what is the reason for the absence of phase separation for small $\omega_0$, 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 $n_i^f/b_i$, of the single-particle gap $\Delta_c$, and of the the TLL parameter $K_\rho$. 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

$$\Delta_c(L) = E(N + 1) + E(N - 1) - 2E(N),$$

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 $\Delta_c$ 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 $K_\rho$ is more promising. Here bosonization field theory predicts how $K_\rho$ should behave at a quantum critical point. In order to determine $K_\rho$ accurately by DMRG,
we first have to calculate the static (charge) structure factor
\begin{equation}
S_c(q) = \frac{1}{L} \sum_{j,l} e^{i q (j-l)} \langle (f_j^\dagger f_j - n)(f_l^\dagger f_l - n) \rangle,
\end{equation}
where the momenta \( q = 2\pi m/L \) with integers \( 0 < m < L \) [17]. The TLL parameter \( K_\rho \) is proportional to the slope of \( S_c(q) \) in the long-wavelength limit \( q \to 0^+ \):
\begin{equation}
K_\rho = \pi \lim_{q \to 0^+} \frac{S_c(q)}{q}.
\end{equation}
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 \( K^{CDW}_\rho = 1/9 \) [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 \( n^f_i \equiv \langle f_i^\dagger f_i \rangle \) and bosons \( n^b_i \equiv \langle b_i^\dagger b_i \rangle \). 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 \( \lambda \)'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 \( \omega_0 \) and \( \lambda \)—the quantum phase transition takes place, we first compute the single-particle gap \( \Delta_c \) and TLL charge exponent \( K_\rho \) for finite chains with up to \( L = 150 \) sites and OBC. Then we perform a finite-size scaling as illustrated for \( K_\rho \) by Fig. 2, left panel. Here open symbols give \( K_\rho \) 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 \( \lambda \)
at fixed $\omega_0 = 2$ the values of $K_\rho$ 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 $2k_F$-CDW insulator with finite charge gap $\Delta_c$. Furthermore, calculating $K_\rho(L)$ for $N = L/3 - 1$ particles, we can show that the infinitesimally doped CDW insulator has $K_\rho^{CDW} = 1/9$ at $n_f = 1/3$. Deep in the CDW phase, $K_\rho$ 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 $K_\rho$ values. Within the TLL region $2/9 < K_\rho < 1$. Of course, the TLL appears at large $\lambda$, when any distortion of the background medium readily relaxes ($\propto \lambda$), or, in the opposite limit of small $\lambda$, 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 $2k_F$-CDW phase with $\Delta_c > 0$ and long-range order appears, at half-filling, for small $\lambda$ and by trend large $\omega_0$ (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 $\lambda$-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 $V_2 = 8t_b^4/3\omega_0^3$, i.e., $V_2/t_f = 4t_b^2/3\lambda \omega_0^2$, 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
the background medium. The metallic phase is a Tomonaga-Luttinger liquid with $2/9 < K_{\rho} < 1$. The insulator represents a $2k_F$ charge density wave with $K_{\rho}^{\text{CDW}} = 1/9$ deep inside the long-range ordered state. Performing a careful finite-size scaling analysis, the phase transition point can be precisely determined by $K_{\rho}$. 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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References

[1] G. Grüner: Density Waves in Solids (Addison Wesley, Reading, MA, 1994).
[2] M. Berciu: Physics 2 (2009) 55.
[3] D. M. Edwards: Physica B 378-380 (2006) 133.
[4] A. Alvermann, D. M. Edwards, and H. Fehske: Phys. Rev. Lett. 98 (2007) 056602.
[5] G. Wellein, H. Fehske, A. Alvermann, and D. M. Edwards: Phys. Rev. Lett. 101 (2008) 136402.
[6] S. Ejima, G. Hager, and H. Fehske: Phys. Rev. Lett. 102 (2009) 106404.
[7] S. Ejima and H. Fehske: Phys. Rev. B 80 (2009) 155101.
[8] H. Fehske, S. Ejima, G. Wellein, and A. R. Bishop: J. Phys.: Conference Series 391 (2012) 012152.
[9] S. Ejima, S. Sykora, K. W. Becker, and H. Fehske: Phys. Rev. B 86 (2012) 155149.
[10] D. M. Edwards, S. Ejima, A. Alvermann, and H. Fehske: J. Phys. Condens. Matter 22 (2010) 435601.
[11] S. Nishimoto, S. Ejima, and H. Fehske: Phys. Rev. B 87 (2013) 045116.
[12] J. M. Kosterlitz and D. J. Thouless: J. Phys. C 6 (1973) 1181.
[13] P. Schmitteckert and R. Werner: Phys. Rev. B 69 (2004) 195115.
[14] S. R. White: Phys. Rev. Lett. 69 (1992) 2863.
[15] E. Jeckelmann and S. R. White: Phys. Rev. B 57 (1998) 6376.
[16] E. Jeckelmann and H. Fehske: Rivista del Nuovo Cimento 30 (2007) 259.
[17] S. Ejima, F. Gebhard, and S. Nishimoto: Europhys. Lett. 70 (2005) 492.
[18] H. J. Schulz: in *Strongly Correlated Electronic Materials*, ed. K. S. Bedell, Z. Wang, and D. E. Meltzer (Addison-Wesley, Reading, MA, 1994), pp. 187; cond-mat/9412036.

[19] T. Giamarchi: *Quantum Physics in One Dimension* (Clarendon Press, Oxford, 2003).