Available online at www.sciencedirect.com
SCIENCE DIRECT®
ELSEVIER
Physica B 359–361 (2005) 699–701
PHYSICA B
www.elsevier.com/locate/physb

Luttinger liquid versus charge density wave behaviour in the one-dimensional spinless fermion Holstein model

H. Fehske[a,*], G. Wellein[b], G. Hager[b], A. Weiße[c], K.W. Becker[d], A.R. Bishop[e]

[a]Institut für Physik, Universität Greifswald, D-17487 Greifswald, Germany
[b]Regionales Rechenzentrum Erlangen, Universität Erlangen-Nürnberg, Germany
[c]School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia
[d]Institut für Theoretische Physik, TU Dresden, D-01062 Dresden, Germany
[e]Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Abstract

We discuss the nature of the different ground states of the half-filled Holstein model of spinless fermions in 1D. In the metallic regime we determine the renormalised effective coupling constant and the velocity of the charge excitations by a density-matrix renormalisation group (DMRG) finite-size scaling approach. At low (high) phonon frequencies the Luttinger liquid is characterised by an attractive (repulsive) effective interaction. In the charge-density wave Peierls-distorted state the charge structure factor scales to a finite value indicating long-range order.

PACS: 71.10.Hf; 71.38.−k; 71.45.Lr

Keywords: Non-Fermi liquid behaviour; Quantum phase transition; Mott–Hubbard systems

The challenge of understanding quantum phase transitions in novel quasi-1D materials has stimulated intense work on microscopic models of interacting electrons and phonons such as the Holstein model of spinless fermions (HMSF)

$$H = -t\sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + \omega_0 \sum_i b_i^\dagger b_i - g\omega_0 \sum_i (b_i^\dagger + b_i)(n_i - \tfrac{1}{2}). \quad (1)$$

The HMSF describes tight-binding band electrons coupled locally to harmonic dispersionless optical phonons, where t, ω_0, and g denote the electronic transfer amplitude, the phonon frequency, and the electron–phonon (EP) coupling constant, respectively.

*Corresponding author. Tel.: +49 3834 86 4760; fax: +49 3834 86 4701.
E-mail address: fehske@physik.uni-greifswald.de (H. Fehske).

0921-4526/$ - see front matter © 2005 Elsevier B.V. All rights reserved.
doi:10.1016/j.physb.2005.01.198

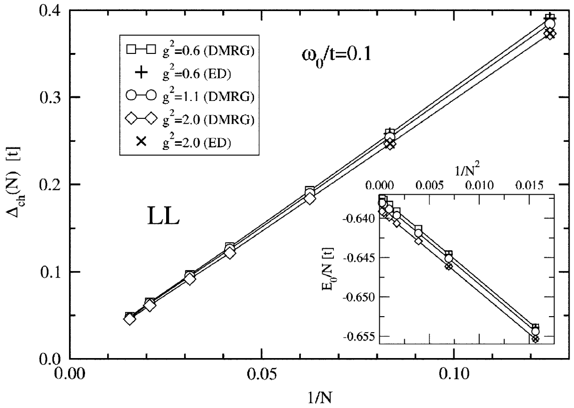

Fig. 1. Finite-size scaling of the charge gap $\Delta_{\rm ch}(N)$ and the ground-state energy $E_0(N)$. Exact diagonalisation (ED) data is included for comparison.

Table 1
LL parameters at small and large phonon frequencies

g^2	$\omega_0/t = 0.1$		$\omega_0/t = 10.0$	
	K_ρ	$u_\rho/2$	K_ρ	$u_\rho/2$
0.6	1.031	~ 1	~ 1	0.617
2.0	1.055	0.995	0.949	0.146
4.0	1.091	0.963	0.651	0.028

Despite its simplicity the HMSF is not exactly solvable and a wide range of numerical methods has been applied in the past to map out the ground-state phase diagram in the g–ω_0 plane, in particular for the half-filled band case ($N_{\rm el} = N/2$). There, the model most likely exhibits a transition from a Luttinger liquid (LL) to a charge-density wave (CDW) ground state above a critical EP coupling strength $g_c(\omega_0) > 0$ [1].

In this contribution we present large-scale DMRG calculations, providing unbiased results for the (non-universal) LL parameters u_ρ, K_ρ, and the staggered charge structure factor $S_c(\pi)$.

To leading order, the charge velocity u_ρ and the correlation exponent K_ρ might be obtained from a finite-size scaling of the ground-state energy of a finite system $E_0(N)$ with N sites

$$\varepsilon_0(\infty) - (E_0(N)/N) = (\pi/3)(u_\rho/2)/N^2 \quad (2)$$

($\varepsilon_0(\infty)$ denotes the bulk ground-state energy density) and the charge excitation gap

$$\Delta_{\rm ch}(N) = E_0^{(\pm 1)}(N) - E_0(N) = \pi(u_\rho/2)/(NK_\rho) \quad (3)$$

(here $E_0^{\pm 1}(N)$ is the ground-state energy with ± 1 fermions away from half-filling). The LL scaling relations (2) and (3) were derived for the pure electronic spinless fermion model only [2].

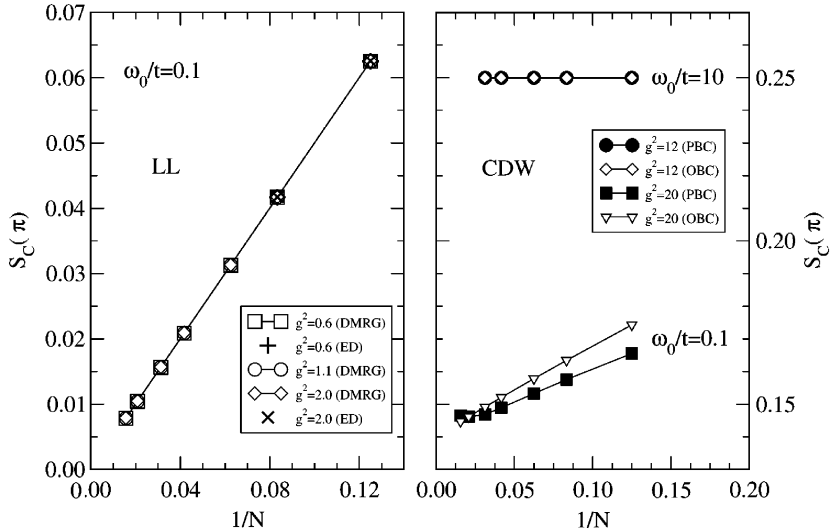

Fig. 2. Scaling of the charge structure factor $S_c(\pi)$ using periodic (PBC) and open (OBC) boundary conditions.

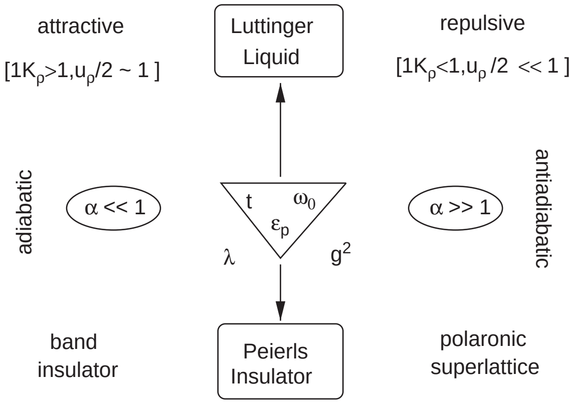

Fig. 3. Phase diagram of the 1D half-filled spinless fermion Holstein model. Here $\alpha = \omega_0/t$, $\varepsilon_p = \omega_0 g^2$, and $\lambda = \varepsilon_p/2t$.

Fig. 1 demonstrates, exemplarily for the adiabatic regime, that they also hold for the case that a finite EP coupling is included. The resulting LL parameters are given in Table 1. Most notably, around $\omega_0/t \sim 1$, the LL phase splits in two different regimes: For small phonon frequencies the effective fermion–fermion interaction is *attractive*, while it is *repulsive* for large frequencies. In the latter region the kinetic energy is strongly reduced and the charge carriers behave like (small) polarons. In between, there is a transition line $K_\rho = 1$, where the LL is made up of (almost) non-interacting particles. The LL scaling breaks down just at $g_c(\omega/t)$, i.e. at the transition to the CDW state. We found $g_c^2(\omega/t = 0.1) \simeq 7.84$ and $g_c^2(\omega/t = 10) \simeq 4.41$ [3].

Fig. 2 proves the existence of the long-range ordered CDW phase above g_c. Here the charge structure factor

$$S_c(\pi) = \frac{1}{N^2} \sum_{i,j} (-1)^j \langle (n_i - \tfrac{1}{2})(n_{i+j} - \tfrac{1}{2}) \rangle \qquad (4)$$

unambiguously scales to a finite value in the thermodynamic limit ($N \to \infty$). Simultaneously $\Delta_{ch}(\infty)$ acquires a finite value. In contrast we have $S_c(\pi) \to 0$ in the metallic regime ($g < g_c$). The CDW for strong EP coupling is connected to a Peierls distortion of the lattice, and can be classified as traditional band insulator and bipolaronic insulator in the strong-EP coupling adiabatic and anti-adiabatic regimes, respectively.

The emerging physical picture can be summarised in the schematic phase diagram shown in Fig. 3. In the adiabatic limit ($\omega_0 \to 0$) any finite EP coupling causes a Peierls distortion. In the anti-adiabatic strong EP coupling limit ($\omega_0 \to \infty$), the HMSF can be mapped perturbatively onto the XXZ model and the metal–insulator transition is consistent with a Kosterlitz–Thouless transition at $g_c^2(\infty) \simeq 4.88$.

Work was supported by DFG under SPP 1073 and SFB 463, KONWIHR, HLRN Berlin, and the US DOE.

References

[1] See, e.g., R.B. Bursill, R.H. McKenzie, C.J. Hamer, Phys. Rev. Lett. 80 (1998) 5607;
S. Sykora, A. Hübsch, K.W. Becker, G. Wellein, H. Fehske, Phys. Rev. B 71 (2005) 045112, and references therein.
[2] J.L. Cardy, J. Phys. A 17 (1984) L385;
J. Voit, Rep. Prog. Phys. 58 (1995) 977.
[3] H. Fehske, M. Holicki, A. Weiße, Adv. Solid State Phys. 40 (2000) 235.