DMRG analysis of the SDW-CDW crossover region in the 1D half-filled Hubbard-Holstein model

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Abstract. In order to clarify the physics of the crossover from a spin-density-wave (SDW) Mott insulator to a charge-density-wave (CDW) Peierls insulator in one-dimensional (1D) systems, we investigate the Hubbard-Holstein Hamiltonian at half filling within a density matrix renormalisation group (DMRG) approach. Determining the spin and charge correlation exponents, the momentum distribution function, and various excitation gaps, we confirm that an intervening metallic phase expands the SDW-CDW transition in the weak-coupling regime.

The Hubbard-Holstein model (HHM) [1] is archetypal for exploring the complex interplay of electron-electron and electron-phonon interactions especially in quasi-1D materials, such as halogen-bridged transition metal complexes, charge transfer salts, or organic superconductors [2]. It accounts for a tight-binding electron band ($\propto 2t$), an intra-site Coulomb repulsion between electrons of opposite spin ($\propto u = U/4t$), a local coupling of the charge carriers to optical phonons ($\propto \lambda = g^2\omega_0/2t$), and the energy of the phonon subsystem in harmonic approximation ($\propto \omega_0/t$):

$$\mathcal{H} = -t \sum_{j\sigma}(c_{j\sigma}^\dagger c_{j+1\sigma} + \text{h.c.}) + U \sum_j n_{j\uparrow}n_{j\downarrow} - g\omega_0 \sum_{j\sigma}(b_j^\dagger + b_j)n_{i\sigma} + \omega_0 \sum_j b_j^\dagger b_j. \tag{1}$$

Here $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) a spin-σ electron at Wannier site i of an 1D lattice with N sites, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, and $b_i^\dagger$ (b_i) are the corresponding creation (annihilation) operators for a dispersionless phonon. We consider the case $\frac{1}{N}\sum_{i\sigma} n_{i\sigma} = 1$ hereafter, and take t as energy unit.

Based on exact diagonalisation data for the staggered static spin/charge structure factor, $S_{\sigma/\rho}(q) = \frac{1}{N}\sum_{j,\ell} e^{iq(j-\ell)}\langle(\hat{n}_{j\uparrow} \pm \hat{n}_{j\downarrow})(\hat{n}_{\ell\uparrow} \pm \hat{n}_{\ell\downarrow})\rangle$, it has been argued that the HHM shows a crossover between Mott and Peierls insulating phases near $u/\lambda \simeq 1$ [3]. But this only holds in the strong-coupling adiabatic-to-intermediate phonon frequency regime. Later on the ground-state phase diagram of the HHM was explored in more detail, also for weak interaction strengths and large phonon frequencies. In this regime, variational displacement Lang-Firsov [4], stochastic series expansion QMC [5], and DMRG [6] methods give strong evidence that, if λ is enhanced at fixed u and ω_0, the SDW-CDW transition splits into two subsequent SDW-metal and metal-CDW transitions at λ_{c1} and λ_{c2}, respectively (see fig. 1, dashed and dot-dashed lines). Very recent DMRG data indicated that in the anti-adiabatic regime of very large phonon frequencies the metallic phase might be even more extended than the one obtained by QMC and is subdivided into regions with a normal 1D metallic (I) and a bipolaronic-liquid (II) behaviour [7].

In this work, we will re-examine the weak-coupling SDW-CDW transition regime by calculating the ground-state properties of the HHM in the framework of a large-scale numerical (boson pseudo-site) DMRG approach supplemented by a finite-size scaling analysis [8].
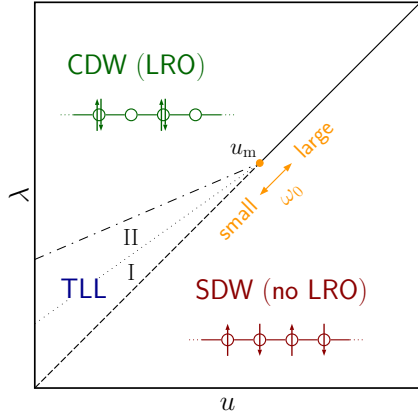
Figure 1. Qualitative phase diagram of the 1D Hubbard-Holstein model. Given that in the half-filled HHM model the ground-state is metallic at $u = 0$ for $\omega_0 > 0$ provided that $g < g_c$, it was proposed that this metallic phase continues to exist between the SDW and CDW states for $u > 0$ [4, 5, 6, 7]. With increasing ω_0 the region of the intervening metallic state increases, and the tricritical point u_m moves to larger u [5]. The SDW state shows no long-range order (LRO) and is characterised by a vanishing spin gap Δ_s but a finite charge gap Δ_{c_1}, whereas the CDW phase exhibits true LRO and $\Delta_s = \Delta_{c_1} > 0$.

Characterising the SDW-CDW-intervening metallic phase of the HHM, we presume that for the metallic state a Tomonaga-Luttinger-liquid (TLL) description holds. In the TLL picture, nonuniversal coefficients, K_ρ and K_σ, determine the decay of correlation functions and therefore can be used to identify the properties of the TLL phase [9], but also the phase boundaries to the insulating states [5]. In practice, we can extract the TLL correlation exponents from the slope of the corresponding structure factors in the long-wavelength limit [5, 10]: $K_{\rho/\sigma} = \pi \lim_{q \to 0} S_{\rho/\sigma}(q)/q$, where $q = 2\pi/N$ for $N \to \infty$.

Specifically, $K_\rho > 1$ ($K_\rho < 1$) corresponds to attractive (repulsive) charge correlations in the TLL and $K_\rho = 0$ signals an insulating phase. Hence K_ρ jumps from $1 \to 0$ at the metal-SDW/CDW transitions. The spin exponent takes the value $K_\sigma = 0$ in a spin-gapped phase and $K_\sigma = 1$ everywhere else in the thermodynamic limit [11]. For finite systems the situation is more involved, in particular for the spin exponent K_σ. First, the convergence $K_\sigma \to 0$ is slow-going as $N \to \infty$ in the spin-gapped phase. Second, logarithmic corrections prevent $K_\sigma \to 1$ in the spin-gapless (SDW) phase. On the other hand, these logarithmic corrections vanish at the critical point, where the spin gap opens, and we can utilise that K_σ (K_ρ) crosses 1 from above (below) at some λ_{c_1} (as the electron-phonon coupling increases for fixed u), in order to determine the SDW-metal phase boundary itself. Increasing λ further, K_ρ should cross 1 once again, this time from above, at another critical coupling strength, λ_{c_2}, which pins the metal-CDW transition point down.

Figure 2 corroborates this scenario for the anti-adiabatic regime of the HHM. The two critical values λ_{c_1} and λ_{c_2} are in accord with the phase diagram obtained by QMC [5]. $K_\sigma < 1$ and $K_\rho > 1$ earmark the intervening metallic phase. In terms of the TLL framework, a metallic phase with $K_\rho > 1$ exhibits dominant superconducting correlations. Recent DMRG calculations of the the (s–, p–, and d–wave) superconducting correlation functions of the half-filled HHM indicate, however, that these correlations are only sub-dominant against CDW correlations [6], while QMC investigations attributed the $K_\rho > 1$ to finite-size effects and suggest that $K_\rho(N \to \infty) = 1$, i.e., superconducting and CDW correlations are exactly degenerate.

Here we inspect the finite-size scaling of the spin and single-particle charge excitation gaps, $\Delta_s(N) = E_0(1) - E_0(0)$ and $\Delta_{c_1}(N) = E_0^+(1/2) + E_0^-(-1/2) - 2E_0(0)$, respectively, as well as that of the two-particle binding energy $\Delta_b(N) = E_0^{2-}(0) + E_0(0) - 2E_0^-(-1/2)$, where $E_0^{(L\pm)}(S^z)$ is the ground-state energy at or away from half-filling with $N_e = N \pm L$ particles in the sector with total spin-z component S^z. The left panel of fig. 2 shows that both spin and charge gaps open at λ_{c_1} (but there is no LRO). For $u < u_m$, the transition at λ_{c_1} seems to be of Kosterlitz-Thouless type, i.e. just above λ_{c_1} the gaps are exponentially small and therefore their magnitude is difficult to determine. In this region, denoted by (I) in fig. 1, we find $\Delta_{c_1} \sim \Delta_s$,
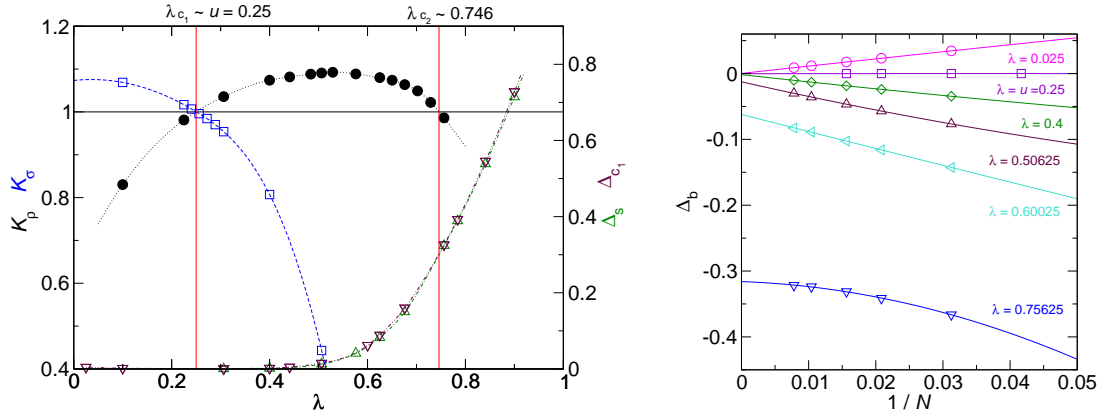
Figure 2. DMRG results for the half-filled HHM with $u = 0.25$ and $\omega_0 = 5$. Left panel: charge (K_ρ, filled circles) and spin (K_σ, open squares) TLL exponents as functions of λ [left-hand axis of ordinate]. Open triangles up (triangles down) give the spin (charge) gap Δ_s (Δ_{c_1}) [right-hand axis of ordinate]. Data shown are extrapolated values for the infinite systems, using open boundary conditions. Right panel: Finite-size scaling of the binding energy Δ_b for different λ; lines are polynomial fits. In the numerical calculations we use up to five pseudo-sites and keep 2400 density-matrix eigenstates; then, for all parameters studied, the local boson density is less than 10^{-8} and the discarded weight is smaller than 10^{-9}.

and the binding energy Δ_b is also extremely small, or maybe even zero (see triangles up, right-hand panel of fig. 2). As λ increases, we obtain a (smooth) crossover to a metallic regime with a noticeable two-particle binding $\Delta_b < 0$ (region (II) in fig. 1), where $\Delta_{c_1} \sim \Delta_s$. This is in accord with the very recent findings of Ref. [7], where a subdivision of the metallic phase into a weakly renormalised TLL (I) and a bipolaronic liquid[1] (II) was suggested. In the latter phase, the two-particle excitation gap $\Delta_{c_2}(N) = E_0^{2+}(0) + E_0^{2-}(0) - 2E_0(0)$ was shown to scale to zero. In the CDW phase, which typifies a bipolaronic superlattice at large phonon frequencies, we have, besides $\Delta_s = \Delta_{c_1} > 0$, $\Delta_{c_2} > 0$ and $\Delta_b < 0$, whereas in the SDW state $\Delta_{c_2} > 0$ but $\Delta_b(N \to \infty) \to 0$. While the basic scenario discussed so far persists in the adiabatic regime, the metallic region shrinks as the phonon frequency ω_0 becomes smaller [5, 7]. Furthermore, the CDW state rather behaves as a normal Peierls insulator and consequently there is a weaker tendency towards bipolaron formation in the metallic state for small λ, and $u < u_m$.

Finally, let us investigate the behaviour of the momentum distribution function, $n_\sigma(k) = \frac{1}{N} \sum_{j,l=1}^{N} \cos(k(j-l)) \langle c_{j,\sigma}^\dagger c_{l,\sigma} \rangle$, $k = 2\pi m/N$, $m = 0, \dots, N/2$, which can be obtained by DMRG for a system with periodic boundary conditions.

Figure 3 shows the variation of $n(k)$ for weak (circles) and intermediate (stars) Hubbard interactions in the SDW (a), TLL (b)-(c), and CDW (d) phases. The momentum distribution is a monotonously decreasing function as k changes from the centre ($k = 0$) to the boundary of the Brillouin zone ($k = \pi$). Since we consider the weak-coupling regime, $n(k)$ is only weakly renormalised away from the Fermi momentum k_F. For a 1D TLL, instead of the Fermi liquid typical jump of $n(k)$ at k_F, one finds an essential power-law singularity [9], corresponding to a vanishing quasiparticle weight $Z = 0$. For finite TLL systems, the difference $\Delta = n(k_F - \delta) - n(k_F + \delta)$ is finite (with $\delta = \pi/N = \pi/66$ in our case), and rapidly decreases with increasing couplings λ, u. Approaching the insulating SDW/CDW states $n(k)$ becomes a smooth curve, i.e. the singularity vanishes and $\Delta \to 0$. At very large λ, the system develops a

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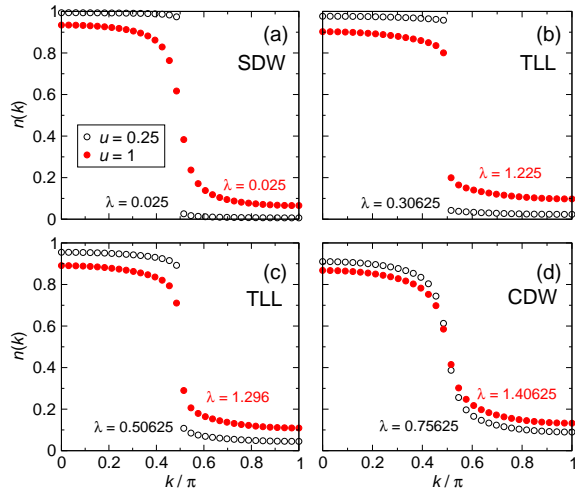[1] Note that the polaronic two-particle bound states are not necessarily small (i.e. on-site).

Figure 3. Momentum distribution of the half-filled HHM in the anti-adiabatic regime ($\omega_0 = 5$). Open (closed) circles give DMRG results at $u = 0.25$ ($u = 1$) for a system with $N = 66$ sites and periodic boundary conditions. The occupation of fermionic states carrying momentum k is given by $n(k) = \frac{1}{2} \sum_\sigma n_\sigma(k)$, and we have $k_F = \pi/2$, $n_{k_F} = 1/2$ for the half-filled band case. In the intermediate metallic phase, $n(k)$ exhibits a power-law singularity at k_F [see panels (b) and (c)]. At weak and strong electron-phonon couplings insulating SDW [panel (a)] and CDW [panel (d)] are realised, respectively.

"perfect" CDW with $n(k) = 1/2$ for all momenta k.

To summarise, we validated the existence of an intervening metallic phase in the SDW-CDW transition regime of the 1D half-filled Hubbard-Holstein model for $u < u_m$ by large-scale DMRG calculations. Spin and charge gaps open exponentially slowly at the SDW-TLL transition point, λ_{c_1}, but no long-range order develops. $\lambda_{c_1}(u, \omega_0)$ can be determined from the "1"–crossing of the spin and charge TLL parameters. In the TLL, the momentum distribution function exhibits a power-law singularity at k_F. As the electron-phonon coupling increases, a crossover to a bipolaronic metal, indicated by negative binding energy, takes place, before the systems enters the long-range ordered insulating CDW phase at a second critical coupling λ_{c_2}. We would like to point out that fixing the metal-CDW phase boundary quantitatively is a difficult issue.

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