Fractionally charged excitations in the charge density wave state of a quarter-filled \( t \)-\( J \) chain with quantum phonons

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Abstract. Elementary excitations of the 4\( k_F \) charge density wave state of a quarter-filled strongly correlated electronic one-dimensional chain are investigated in the presence of dispersionless quantum optical phonons using Density Matrix Renormalization Group techniques. Such excitations are shown to be topological solitons carrying charge \( e/2 \) and spin zero. Relevance to the 4\( k_F \) charge density wave instability in (DI – DCNQI)\textsubscript{2}\( \text{Ag} \) or recently discovered in (TMTTF)\textsubscript{2}X (\( X = \text{PF}_6, \text{AsF}_6 \)) is discussed.

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1 Introduction

It is well known that one-dimensional (1D) Su-Shrieffer-Heeger (SSH) [1] or Hubbard-SSH models exhibit exotic elementary excitations including neutral soliton with spin \( \frac{1}{2} \), charged soliton with spin zero (\( \frac{1}{2} \)-filled band) [2] as well as fractionally charged soliton (\( \frac{1}{2} \) and \( \frac{1}{4} \)-filled band) [3,4]. In these models, the phonons couple to the electrons \( \text{via} \) inter-site interactions which lead to an insulating (CDW) state. In fact, such solitonic excitations are also generic in commensurate site-centered Charge Density Wave (CDW) states and, hence, should also exist (in the vicinity of commensurate fillings) in the case of strong short range electronic repulsion leading to commensurate 4\( k_F \) charge instability. In addition to strong electron-electron correlation, local on-site electron-phonon (e-ph) coupling (to be compared with the inter-site vibration in the SSH model) is of particular relevance in systems where the “site” represents a complex structure with internal degrees of freedom. Molecular crystals such as the quasi-1D charge transfer salts [5] present this type of characteristic. Interplay between electron-electron and e-ph interactions provides a very rich physics. For example, several systems have been recently observed to present transitions towards charge ordered phases where the molecules of the conducting stack support unequal electron densities, and in some cases associated relaxation of their internal geometry. This is for instance the case for the most strongly 1D system of the Bechgaard-Fabre salts family, namely (TMTTF)\textsubscript{2}\( \text{PF}_6 \) and (TMTTF)\textsubscript{2}\( \text{AsF}_6 \); below the Mott localization temperature \( T_L \) evidences for an additional transition towards a 4\( k_F \) (site-centered) CDW state have been recently provided by dielectric response measurements [6], NMR [7] and anomalous temperature dependence of the X-ray Bragg peaks [8]. Similar transitions have been seen in (BEDT – TTF)\textsubscript{2}X [9] as well as in (DI – DCNQI)\textsubscript{2}\( \text{Ag} \) [10] which exhibits below 220 K a 4\( k_F \) CDW associated with geometry modulations of the DI – DCNQI molecules.

A pictorial description of a solitonic state can be simply given assuming \( \text{e.g.} \) a quarter-filled strongly correlated chain, in a 4\( k_F \) CDW state, provided a doubling of the unit cell. In that case, the GS charge modulation can be parametrized as \( \langle n_i \rangle = \frac{1}{4} + A_{4k_F} \cos(4k_Fr_i + \phi) \) where \( k_F = \pi/4, A_{4k_F} \) is the magnitude and \( \phi \) the phase of the charge oscillation. Hence, due to the equivalence between the even and odd sites, the GS is two fold degenerate (\( \phi = 0 \) and \( \phi = \pi \)). A solitonic excitation can be described as a state which interpolates between the two different GS patterns with a slowly monotonically varying phase \( \phi(r_i) \) from let’s say 0 at \( r_i \to -\infty \) to \( \pi \) when \( r_i \to +\infty \). Simple counting arguments show, in fact, that such an excitation carries a charge \( Q = \pm \frac{e}{2} \) and, therefore, can be generated by doping the commensurate CDW GS.

In this paper, we investigate the role of quantum local phononic (optical) modes on the formation and on the stability of the solitonic excitations occurring in an insulating 4\( k_F \) CDW phase of a quarter-filled strongly correlated electronic chain. This issue is of particular interest since a coupling to local phonons might affect the physics of the solitons (such as its width, its interaction, etc...). Numerical results will be obtained by the Density Matrix Renormalization Group (DMRG) method applied to open or cyclic chain segments carrying no, a single or two solitonic excitations.
2 Model

The following analysis is based on the 1D \( t-J-V \)-Holstein model at quarter filling. This model describing strongly correlated electrons coupled to dispersionless phonons can be written as \( H = H_c + H_{e-ph} \) with

\[
H_c = \sum_{i,\sigma} \left( c_{i+1,\sigma}^\dagger c_{i,\sigma} + h.c. \right) + J \sum_i S_i \cdot S_{i+1} + V \sum_i n_i n_{i+1}
\]

\[
H_{e-ph} = \sum_i n_i \left( b_i^\dagger + b_i \right) + \omega \sum_i \left( b_i b_i + 1/2 \right)
\]

where \( c_{i,\sigma}, c_{i,\sigma}^\dagger \) are projected creation and annihilation operators of electrons of spin \( \sigma \) at sites \( i \) (doubly occupied sites are projected out, the strong correlation limit is therefore assumed), \( n_i \) is the electron number and \( S_i \) is the spin operator at site \( i \). \( b_i^\dagger \) and \( b_i \) are the local phonons creation and annihilation operators. The energy scale is fixed by \( \hbar = 1 \). Note that the phononic part can be re-written as

\[
\omega \left( b_i^\dagger + n_i \frac{\omega}{2} \right) \left( b_i + n_i \frac{\omega}{2} \right) + \text{const.}
\]

showing that the coupling of the on-site vibrations to the electrons induces displacements of the oscillator proportional to the site charge. In fact, this term mimics the relaxation of the internal geometry of a site as a function of its ionicity.

Before proceeding further, it is interesting to examine the adiabatic limit. Absorbing the e-ph coupling \( g \) in the definition of the (classical) on-site displacement \( g(b_i^\dagger + b_i) \rightarrow \delta_i \), the phononic part takes the form of a classical elastic energy \( \frac{1}{2} K \sum_i \delta_i^2 \). The magnitude of the e-ph coupling is then given by a single parameter, the inverse lattice stiffness \( K^{-1} = 2g^2/\omega \). Hence, the adiabatic limit is reached assuming the following limits: \( \omega \rightarrow 0 \), \( g \rightarrow 0 \) and \( K^{-1} \rightarrow \text{const.} \). The phase diagram of this model has been investigated recently by Riera and Poilblanc [12]. It is well known that a quarter-filled infinite-\( U \) (i.e. \( J = 0 \)) model exhibits a 4\( k_F \) CDW (Mott-Hubbard like) instability only when the nearest neighbor (NN) repulsion \( V \) exceeds 2 [11]. This instability is in fact enhanced by the lattice coupling and the 4\( k_F \) CDW phase becomes stable even when \( V < 2 \) and \( J \) finite for \( K^{-1} \) exceeding a \( V \)-dependent critical value [12]. The numerical study of the model with quantum phonons using the infinite system DMRG method [13] requires an approximate (but reliable) treatment of the phonon degrees of freedom [14–16]. Indeed, an infinite number of phononic quantum states lives on each site. In order to render the calculations feasible, the basis set has been truncated on each site to the two lowest vibronic states. This choice is physically reasonable as long as the frequency \( \omega \) is not too small since only the lowest vibronic states are expected to be involved [16]. In all cases, we kept \( m = 216 \) states per renormalized block. We have chosen parameters like \( V = 1 \) and \( J = 0.3 \) which are generic for strongly correlated 1D materials. For such parameters, the adiabatic GS is a 4\( k_F \) CDW for \( K^{-1} > K_{\text{crit}}^{-1} \approx 1.1 \). GS and solitonic states of the system have been investigated as a function of \( K^{-1} \).

In order to determine the phase diagram at quarter-filling, we have computed the charge gap \( \Delta_p = E_0(2N, N+1) + E_0(2N, N-1) - 2E_0(2N, N) \) (where \( E_0(N_c, N_s) \) is the GS energy of \( N_c \) electrons on \( N_s \) sites).

3 Results and discussion

Figure 1 shows the schematic phase diagram as a function of \( g/\omega \) and \( K^{-1} \) exhibiting a 4\( k_F \) CDW insulating phase and a uniform metallic phase with usual Luttinger liquid characteristics (in particular the power law decrease of the charge and spin correlation functions). It has been argued that, although phononic quantum fluctuations are present, such state still belongs to the Luttinger Liquid universality class [14,16]. The insulating 4\( k_F \) CDW phase was characterized both by a finite charge gap and long range staggered charge correlations associated to the finite order parameter \((-1)^j c_n(j)\). Special care is needed for \( \omega \rightarrow 0 \) since, in this case, the truncation of the phonon basis is no more adequate and more phonon states are expected to be excited. Indeed, \( K_{\text{crit}}^{-1} \approx 1.1 \) obtained in the adiabatic approximation [12] does not seem to appear as an asymptotic limit for the metal-insulator boundary when \( \omega \rightarrow 0 \) and \( g/\omega \rightarrow +\infty \). Within our treatment, \( K_{\text{crit}}^{-1} \) tends towards zero, which seems inconsistent with the finite value \( K_{\text{crit}}^{-1} \approx 1.1 \) obtained in the adiabatic approximation [12] for the same \( J \) and \( V \) values. Therefore, we shall restrict in the following analysis to \( \omega > 0.1 \) where we expect our results to be fully reliable.

Let us now discuss the effect of the frequency \( \omega \) at fixed \( K^{-1} \): for values of \( K^{-1} \) such as the adiabatic GS is in

![Fig. 1. Schematic phase diagram of a 1/4-filled \( t-J \) chain for \( J/t = 0.3 \) and \( V/t = 1 \) as a function of \( K^{-1} = 2g^2/\omega \) and \( g/\omega \). The two shaded regions correspond to insulating 4\( k_F \) CDW phases, the dark-shaded one corresponding to the saturated 4\( k_F \) CDW phase : \( A_{2k_F} \geq 1/2 \). The slanted region corresponds to the Luttinger liquid uniform phase. The solid lines, extrapolated by dashed lines correspond to iso-gaps curves, the dotted lines correspond to iso-frequencies curves. The numbers correspond to the width, \( \xi \), of the solitons at the reported points.](image-url)