Charge-density waves in the Hubbard chain: evidence for $4k_F$ instability

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Charge density waves in the Hubbard chain are studied by means of finite-temperature Quantum Monte Carlo simulations and Lanczos diagonalizations for the ground state. We present results both for the charge susceptibilities and for the charge structure factor at densities $\rho = 1/6$ and $1/3$; for $\rho = 1/2$ (quarter filled) we only present results for the charge structure factor. The data are consistent with a $4k_F$ instability dominating over the $2k_F$ one, at least for sufficiently large values of the Coulomb repulsion, $U$. This can only be reconciled with the Luttinger liquid analyses if the amplitude of the $2k_F$ contribution vanishes above some $U^*(\rho)$.

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Charge-density waves (CDW’s) are present in a variety of strongly correlated electron systems, ranging from quasi-one-dimensional organic conductors to the more recently discovered manganites. In order to understand the influence of CDW formation on magnetic order and transport properties, a crucial issue is to establish the period of charge modulation in the ground state. This period, in turn, is primarily determined by the interplay between electron-phonon and electron-electron couplings. For the specific example of quasi-one-dimensional organic conductors at quarter-filled band, both period-2 and period-4 modulations have been observed; these correspond, respectively, to $4k_F$ and $2k_F$, where $k_F = \pi \rho/2$ is the Fermi wave vector for a density $\rho$ of free electrons on a periodic lattice. The use of simplified effective models capturing the basic physical ingredients should therefore be extremely helpful in predicting the dominant instability. In this context, the Hubbard model can be thought of as a limiting case (of vanishing electron-phonon interaction), in which the influence of electronic correlations on CDW modulation can be monitored. However, even for this simplest possible model there has been a disagreement between analyses of the continuum (Luttinger liquid) version and early finite temperature (world-line) quantum Monte Carlo (QMC) simulations. According to the former, the large-distance behaviour of the charge density correlation function is given by

$$
\langle n(x)n(0) \rangle = \frac{K_\rho}{(\pi x)^2} + A_1 \frac{\cos(2k_Fx)}{x^{1+K_\rho} \ln^{3/2} x} + A_2 \frac{\cos(4k_Fx)}{x^{4K_\rho}},
$$

where the amplitudes $A_1$ and $A_2$, and the exponent $K_\rho$ are interaction- and density-dependent parameters; for repulsive interactions $\frac{1}{2} \leq K_\rho < 1$, so that charge correlations are expected to be dominated by the $2k_F$ term. By contrast, the simulations pointed towards $4k_F$ being the main correlations. Nonetheless, based on a Renormalization Group (RG) analysis, it was argued that the $2k_F$ instability should eventually dominate over the $4k_F$ one for sufficiently low temperatures. For infinite coupling the system becomes effectively a spinless fermion problem with a $4k_F$ instability and there is no disagreement in this case.

Since present day computational capabilities allow one to reach much lower temperatures and larger system sizes than before, a numerical reanalysis of the model is certainly in order. Our purpose here is to present the results of such a study. The Hubbard Hamiltonian reads

$$
\mathcal{H} = -t \sum_{i,\sigma} c_i^\dagger c_{i+1,\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow},
$$

where, in standard notation, $U$ is the on-site Coulomb repulsion; the hopping integral sets the energy scale, so we take $t = 1$ throughout this paper. We probe finite temperature properties through determinantal QMC simulations for the grand-canonical version of $\mathcal{H}$, $\mathcal{H}_G = \mathcal{H} - \mu N$, where $\mu \equiv \sum_{\sigma} n_{i\sigma}$, the chemical potential is adjusted to yield the desired particle density. This analysis is supplemented by zero temperature calculations: the ground state of Eq. (3), for finite lattices of $N_s$ sites with periodic boundary conditions, is obtained through the Lanczos algorithm in the subspace of fixed particle-density (canonical ensemble).

The signature of a CDW instability is a peak at $q = q^*$ in the zero-temperature limit of the charge-density susceptibility,

$$
N(q) = \frac{1}{N_s} \int_0^\beta d\tau \sum_{i,\ell} \langle n_i(\tau)n_{i+\ell}(0) \rangle \ e^{iq\ell},
$$

where the imaginary-time dependence of the operators is given by $n_i(\tau) = e^{i\hat{H}\tau} n_i e^{-i\hat{H}\tau}$, with $n_i = n_{i\uparrow} + n_{i\downarrow}$. We recall that in simulations ‘time’ is discretized in intervals $\Delta \tau$, such that the size along this direction is $L = \beta/\Delta \tau$. The CDW instability should also show up as a cusp, again at $q = q^*$, in the zero-temperature charge-density structure factor,
\[ C(q) = \frac{1}{N_s} \sum_{i,\ell} \langle 0 | n_i n_{i+\ell} | 0 \rangle e^{i q \ell}, \]  

where \(|0\rangle\) is the ground state.

Let us first discuss results for an electronic density \(\rho = 1/6\), for which we found that the fermionic determinants in QMC simulations do not suffer from the ‘minus-sign problem’; this allowed us to reach inverse temperatures as large as \(\beta = 25\). From Fig. 1 we see that the \(4k_F\) charge susceptibility appears to be increasing with decreasing temperature, at a rate faster than that at \(2k_F\), especially for \(U = 6\) and 9. The data in Fig. 1 were obtained for \(\Delta \tau = 0.125\), but we have explicitly tested other values to ensure they do not change significantly as \(\Delta \tau \to 0\); each datum point involves typically 20,000 QMC sweeps over all time slices. Further, in order to check if this increase is limited by finite-size or finite-temperature effects, we performed additional simulations on a ‘square space-time lattice’, i.e., we set \(N_s = L\); the result is displayed in Fig. 2 for \(N_s = L \leq 96\). While the charge susceptibility at \(2k_F\) seems to saturate as \(N_s\) increases, the one at \(4k_F\) still scales with \(\ln N_s\), up to the largest sizes considered. Thus, in spite of the very low temperatures reached, we were still unable to find indications of a crossover temperature below which the system is dominated by the \(2k_F\) instability. Also, since \(N_s \propto 1/T\) for the data in Fig. 2, the \(4k_F\) charge susceptibility grows logarithmically with the temperature in this range, similarly to the infinite coupling limit.

We now discuss the charge structure factor at zero temperature, as obtained from Lanczos diagonalizations, still for \(\rho = 1/6\). Figure 3 shows \(C(q)\) for several values of \(U\); for clarity, the curves are shown after suffering successive displacements. For the free case, \(U = 0\), we see a sharp plateau beginning at \(q = 2k_F = \pi/6\), which is the signature of the Peierls instability. This behaviour is quite different from the one observed for \(U \neq 0\); though somewhat rounded for \(U = 2\) and 4, the plateaux now start at \(q = 4k_F = \pi/3\). It is instructive to examine how these roundings evolve with system size. In Fig. 4 we
single out data for \( C(q) \) with \( U = 3 \) and 12, and sizes \( N_s = 12 \) and 24. For each value of \( U \), the data below and above \( 4k_F \) respectively move down and up as \( N_s \) increases, thus sharpening the cusp; in addition, the position of the latter shows no tendency of shifting from \( 4k_F \). Thus, the Lanczos results are consistent with those from QMC simulations, in the sense that a \( 4k_F \) instability is dominant, already for moderate values of \( U \). At this point, it is worth pointing out that the charge structure factor for the Hubbard chain with second neighbour hopping has been calculated through density matrix renormalization group (DMRG). Though their interest was to extract \( K_F \) from the slope of \( C(q) \) at \( q = 0 \), if one reinterprets those data along the lines discussed here, a predominance of the \( 4k_F \) instability can be clearly inferred for the largest values of \( U \) shown in Fig. 11 of Ref. 19. DMRG calculations for the two-leg Hubbard ladder have also led to \( 4k_F \)-like charge correlations.

![Figure 4](image1.png)

**FIG. 4.** Charge structure factor for electron density \( \rho = 1/6 \). Empty squares: \( U = 3, N_s = 12 \); filled squares: \( U = 3, N_s = 24 \); empty circles: \( U = 12, N_s = 12 \); filled circles: \( U = 12, N_s = 24 \). A vertical shift by -0.025 has been imposed on the curves for \( U = 12 \), for clarity.

We now change the band filling to \( \rho = 1/3 \); the average sign of the fermionic determinant is \( \sim 0.9 \) in the worst cases, thus posing no problems to the resulting averages. Figure 3 shows QMC data for the charge susceptibilities with \( U = 6 \) and \( U = 8 \). For \( U = 6 \), an upturn at lower temperatures seems to be setting in for \( 4k_F \), while the \( 2k_F \) data show no noticeable change in growth rate. On the other hand, for \( U = 8 \) the \( 4k_F \) susceptibility grows unequivocally faster with \( \beta \) than the one at \( 2k_F \); see Fig. 6. The corresponding Lanczos data for the charge structure factor are shown in Fig. 6 and, similarly to Fig. 3, the cusp at \( q = 4k_F = 2\pi/3 \) gets visibly sharper as \( U \) increases.

![Figure 6](image2.png)

**FIG. 6.** Charge structure factor for electron density \( \rho = 1/3 \) and \( U = 6 \) (up triangles), 4 (squares), 6 (down triangles), 8 (left triangles), 9 (diamonds), 12 (circles), and 20 (right triangles). The system size is \( N_s = 18 \), and successive vertical shifts by -0.03 have been imposed on the curves, for clarity.

Unfortunately, for larger band fillings the ‘minus-sign problem’ prevents us from reaching very low temperatures. Nonetheless, down to the lowest temperatures probed with acceptable average signs of the fermionic determinant (i.e., \( \langle \text{sign} \rangle \sim 0.7 \) at \( T \sim 1/20 \)), no indications of a \( 2k_F \) peak dominating the charge susceptibility were found for \( \rho = 1/2 \) or \( 3/4 \). Accordingly, the charge structure factor at \( T = 0 \), calculated through Lanczos diagonalizations on a 16-site chain at quarter filling, shown...
in Fig. 4 confirms the previous patterns: there is some rounding near \( q = 4k_F = \pi \), which sharpens as \( U \) increases, consistently with a \( 4k_F \) instability setting in for finite \( U \)’s.

In summary, for all band fillings examined, the charge instability seems to be characterized by a \( 4k_F \) modulation, rather than by \( 2k_F \), at least for \( U \) greater than some \( U^*(\rho) \). The question of how can these findings be reconciled with the analyses of the continuum model still remains. Since Lanczos data have been obtained at zero temperature, and QMC simulations reached much lower temperatures than before, the scenario of a temperature-driven crossover seems now unlikely; it should be recalled that this crossover was predicted based on a weak coupling RG analysis. We therefore envisage the following scenario. While analyses of the Luttinger liquid have so far provided detailed insight into the behaviour of the exponent \( K_F \), little is known about the dependence of the amplitude \( A_1 \) of the \( 2k_F \) contribution [see Eq. (4)] with \( \rho \) and with the coupling constant. Our results may be indicating that, for fixed density \( \rho \), \( A_1 \to 0 \) very fast with increasing \( U \), either exponentially or, less likely, as \( (U^*(\rho) - U)^\psi \), for \( U \leq U^*(\rho) \), with \( \psi > 1 \); a crude examination of the roundings near \( 4k_F \) in the structure factors is consistent with \( U^* \) growing with \( \rho \). An alternative scenario could be that \( 2k_F \) charge correlations in the lattice model would suffer from unusually slow finite-size effects, thus hindering any present day numerical calculations to detect their predominance over the \( 4k_F \) ones; however, since one would need effects slower than those suggested by the logarithmic ‘correction’ in Eq. (4), this scenario is less appealing. Therefore, the presence of a \( 4k_F \) instability can be made compatible with Luttinger liquid picture through the behaviour of the amplitude of the \( 2k_F \) contribution. We hope our results stimulate more extensive work both on the Luttinger liquid and on the lattice model in order to extract a quantitative behaviour for the amplitude \( A_1(\rho, U) \).

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