Charge-density waves in one-dimensional Hubbard superlattices

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Charge-density waves (CDW’s) are present in a variety of homogeneous strongly correlated electron systems, especially some quasi-one-dimensional organic conductors. An interesting property of CDW systems is their non-ohmic behavior: CDW’s incommensurate with the underlying lattice are pinned by impurities, so that only voltages above a certain threshold are able to produce observable currents. Just above this critical voltage, the current rises sharply, indicating a huge increase in the conductivity.

Thus, one of the key issues in the study of CDW’s is to determine the period of charge modulation in the ground state. From the theoretical point of view, this has been addressed with the aid of various models, but care must be taken even in the simplest case of the one-dimensional Hubbard model.

We have recently considered a model for strongly correlated electrons in one-dimensional superlattices defined by the Hamiltonian

$$\mathcal{H} = -t \sum_{i, \sigma} \left( c_i^\dagger \sigma c_{i+1\sigma} + \text{H.c.} \right) + \sum_i U_i n_i^\uparrow n_i^\downarrow$$

where, in standard notation, $i$ runs over the sites of a one-dimensional lattice, $c_i^\dagger \sigma (c_i^\sigma)$ creates (annihilates) a fermion at site $i$ in the spin state $\sigma = \uparrow$ or $\downarrow$, and $n_i = n_i^\uparrow + n_i^\downarrow$, with $n_i^\sigma = c_i^\dagger \sigma c_i^\sigma$; the on-site Coulomb repulsion is taken to be site-dependent: $U_i = U > 0$, for sites within the repulsive layers, and $U_i = 0$ otherwise.

The magnetic properties of model (2) turned out to be quite different from those of the corresponding homogeneous system. Also, the electronic density at which a charge gap opens in these SL’s can be fine-tuned by an appropriate choice of the ‘aspect ratio’ defined as $\ell = L_U/L_0$. The extension of this model to a Luttinger liquid superlattice (LLSL) has been discussed recently.

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We use the Lanczos algorithm to determine the ground state of Eq. (2), for finite lattices of $N_s$ sites with periodic boundary conditions, in the subspace of fixed particle-density (canonical ensemble) $\rho = N_c/N_s$, where $N_c$ is the total number of electrons. The signature of a CDW instability is a cusp at $q = q^*$, in the charge-density structure factor,

$$C(q) = \frac{1}{N_c} \sum_{i,j} e^{i q (r_i - r_j)} \langle Q_i Q_j \rangle ,$$

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with \( \langle Q_i Q_j \rangle = \langle \psi_0 | n_i n_j | \psi_0 \rangle - \langle \psi_0 | n_i | \psi_0 \rangle \langle \psi_0 | n_j | \psi_0 \rangle \), where \( | \psi_0 \rangle \) is the ground state and \( N_c \) is the number of periodic cells, \( N_c = N_s / N_b \), for a basis with \( N_b = L_0 + L_0 \) sites.

In order to study the behavior of \( C(q) \) in the widest possible range of values of \( L_0 \), we focus our discussion on the case of 24-site lattices, with electron density \( \rho = 11/6 \). Figure 1 compares the charge structure factor for the homogeneous chain with that for a SL with \( L_U = 1 \) and \( L_0 = 1 \). From Fig. 1(a) one sees that the \( 2k_F \) cusp in the free (\( U = 0 \)) homogeneous case is displaced to \( 4k_F \) as \( U \) increases. The SL structure changes the periodicity of the CDW as shown in Fig. 1(b): the cusp is displaced relative to the position for the homogeneous chain. Similarly to the homogeneous system, the cusps sharpen as \( U \) increases; their positions, however, remain locked at \( 2 \pi / 3 \) for that SL configuration and electronic density.

Before discussing the location of the cusps, let us check on the role of finite-size effects. Recall that the appropriate finite-size parameter is the number of repeating units, \( N_c \). Figure 2 shows \( C(q) \) for the above mentioned SL and for two different lattice sizes, namely \( N_s = 12 \) \((N_c = 6)\) and \( N_s = 24 \) \((N_c = 12)\). One sees that for \( U = 4 \) the cusp is sharpened as one goes from \( N_c = 6 \) to \( N_c = 12 \); the cusp positions, however, do not change as the size increases. For large couplings \((U = 30 \) in the figure\), the curves lie on top of each other, so that finite-size roundings are not noticeable. Thus we can rule out finite size effects as playing any crucial role in determining the cusp positions.

The main feature determining the periodicity of the CDW can be identified through a systematic study of \( q^* \) as a function of layer thickness. Figure 3 shows the charge structure factor for a fixed length of the repulsive layer \((L_U = 1)\), and for different lengths of the free layer: \( L_0 = 1, 2, 3, \) and \( 5 \). We see that the CDW modulation depends on the superlattice: \( q^*/\pi = 2/3, 1, \) and \( 2/3 \) for \( L_0 = 1, 2, \) and \( 3 \), respectively; the vanishing \( C(q) \) obtained for \( L_0 = 5 \) is associated with \( q^* = 0 \).

These cusp positions can be analysed in a strong coupling scenario. We first recall that there is a special den-
sity, $\rho_I$, corresponding to each free site being doubly occupied, while each repulsive site is singly occupied; it can be written as

$$\rho_I = \frac{2 + \ell}{1 + \ell}.$$  \hspace{1cm} (4)

At this density, a Mott-Hubbard gap opens and the system is an insulator, that is, the transport properties of a SL at $\rho_I$ should be similar to that for a homogeneous chain at half-filling, which includes the breakdown of CDW's. This latter point is nicely illustrated by the vanishing of $C(q)$ for all $q$ for the SL with $L_U = 1$ and $L_0 = 5$, as shown in Fig. 3(d): $\rho_I$ is exactly $11/6$ for that SL. For densities above $\rho_I$, all free sites remain doubly occupied, while the amount of charge on the repulsive sites can fluctuate. Charge correlations between different cells are therefore dominated by the way in which electrons are distributed within each repulsive layer. Accordingly, we define the effective cell density (i.e., the number of active electrons per unit cell),

$$\rho_{\text{eff}} = \rho(L_0 + L_U) - 2L_0,$$  \hspace{1cm} (5)

where $\rho$ is the overall density. If one similarly defines an effective Fermi wave vector, $k_F^*$, from

$$2k_F^* = \pi(2 - \rho_{\text{eff}}),$$  \hspace{1cm} (6)

then the cusp in $C(q)$ is located simply at $q^* = 4k_F^*$, in a way completely analogous to that of the homogeneous system. In Fig. 3(b), $4k_F^*$ thus calculated is indicated by an arrow, and it is clear that it coincides with the cusp positions. By the same token, for all SL’s shown in Fig. 3, the position of the cusps also perfectly match the $4k_F^*$ as obtained from Eq. (6).

It is now illustrative to discuss how the periodicity of the CDW depends on the width of the free layer as the repulsive layer width is kept fixed, as done in Fig. 4, where $q^*$ is shown as a function of $L_0$ for both $L_U = 1$ and $L_U = 2$. First, we see that the strong coupling prediction, $q^* = 4k_F^*$, with $k_F^*$ given by Eq. (6), is satisfied for any $U > 0$: it agrees perfectly well with the data points (circles) obtained from Lanczos diagonalization of different SL’s with $U = 12$. And, second, we see that $q^*$ is periodic with $L_0$, for a fixed $L_U$. The period of oscillation $\Delta L_0$ can be determined by imposing $q^*(L_0) = q^*(L_0 + \Delta L_0)$, which yields

$$\Delta L_0 = (2 - \rho)^{-1} = \frac{\pi}{2k_F^*},$$  \hspace{1cm} (7)

where $\rho$ is the overall density.

A similar oscillatory behavior has been found for the periodicity of SDW’s on Hubbard SL’s which was identified with the exchange oscillation in magnetic multilayers; this latter feature is, in turn, intimately connected with the Giant Magnetoresistance (GMR) effect (see e.g., Ref. 2 and references therein). Thus, the above results indicate that one can also fine-tune a given charge distribution by a suitable choice of the length of the spacer (i.e., free) material.

As a final remark, we should mention that experimental realizations of (variations of) the model discussed here have recently appeared in the literature. Indeed, by growing $L_A$ layers of semimetallic (narrow gap semiconductor) TiSe$_2$ in succession to $L_B$ layers of metallic/superconducting NbSe$_2$ – both compounds undergo CDW transitions – Noh et al. were able to grow ‘superfilms’ 1000 Å thick, with $L_A$ and $L_B$ in the range 1 to 24 layers. The superconducting critical temperature and the temperature dependence of the conductivity were then obtained as functions of the SL structure.

In summary, we have considered the formation of CDW’s in one-dimensional Hubbard superlattices. We have established that the SL structure affects the charge distribution in relation to the homogeneous lattices, though one can still predict the new periodicity through an effective cell density. It has also been established that the periodicity of the CDW is an oscillatory function of the spacer thickness, for a fixed repulsive layer thickness. As a consequence, for a given (overall) electronic density, one can fine-tune a desired charge distribution by a suitable choice of the length of the spacer (i.e., free) material. We hope the present work stimulates further investigations on the superlattices made up of transition metal dichalcogenides, focusing on the CDW periodicity along the direction of growth.

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