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Abstract
We have studied the ground state of one-dimensional Hubbard superlattice structures with
different unit-cell sizes in the presence of an electric field. A self-consistent Hartree–Fock
approximation calculation is done in the weak- to intermediate-interaction regime. Studying the
charge gap at the Fermi level and the charge density structure factor, we get an idea of how the
charge modulation on the superlattice is governed by the competition between the electronic
correlation and the external electric field.

1. Introduction

The study of low-dimensional metallic multilayered structures [1] is interesting because of their unique characteristics. The oscillation of exchange coupling between magnetic layers [2] and the appearance of giant magnetoresistance [3] are among the exciting features of the multilayers. To investigate the properties of the metallic multilayers many theoretical works have been done taking simple superlattice structures as the models [4–8]. This kind of model consists of a periodic arrangement of N_U sites with repulsive on-site Coulomb interaction U (> 0), followed by N_0 sites with no on-site interaction ($U = 0$). Some of these works investigated the ordering [4–7] of the ground state, while others explored the possibility of the metal–insulator transition in these systems [7, 8]. There are possibilities for formation of novel ground states such as charge ordered or spin ordered ones depending on the distribution of the interaction parameter U in such superlattices.

On the other hand, the effect of electric field on strongly correlated low-dimensional electronic systems has attracted much interest in recent years because of their practical applications in tuning dielectric and piezoelectric properties [9]. Many experiments have been done on these low-dimensional systems in the presence of electric field. It was found that spin ordered or charge ordered phases of a Mott insulator collapse in an electric field [10–14]. Also some theoretical works are done on such systems in which a uniform

electric field is implemented in the form of a ramp potential. Applying such an electric field in the homogeneous Hubbard model it was found that the field can induce oscillations in the charge gap of these systems [15, 16]. However, it is not yet known how the superlattice systems behave in the presence of such an electric field.

In this work, we investigate the electronic properties of simple superlattice structures in the presence of electric field. We consider the weak- to intermediate-interaction regime and work under the Hartree–Fock approximation (HFA).

2. The model and the Hartree–Fock approximation

Our model is a one-dimensional N-site Hubbard chain with open boundaries. The model Hamiltonian is

$$H = \sum_i \epsilon_i n_i + t \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.}) + \sum_i U_i n_{i,\uparrow} n_{i,\downarrow}, \quad (1)$$

where $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) is the creation (annihilation) operator for an electron with spin σ ($\uparrow$ or $\downarrow$) at the ith site. $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$, and $n_i = \sum_\sigma n_{i,\sigma}$ is the number operator at the ith site; t is the hopping integral between the nearest neighbor sites. U_i denotes the on-site Coulomb repulsion at the ith site; in a superlattice the U_i follow a repeated pattern depending on the size of the unit cell of the superlattice. ϵ_i is the site energy of the ith site. In the absence of electric field all the ϵ_i are set to
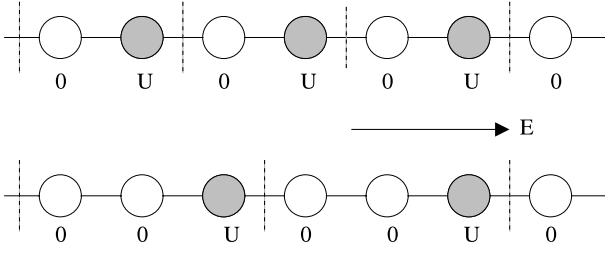
Figure 1. Two different types of superlattice structures studied in the present work. The arrow shows the direction of the electric field.

zero. The external electric field is applied to the system in the form of a ramp potential [15]. In the presence of this field the site energies become

$$\epsilon_i = -\frac{V}{2} + i\frac{V}{N+1},$$

where V is the applied voltage. This form of the site potential is used to ensure that the external bias varies from $-V/2$ to $V/2$ across the superlattice. We will work in the weak to intermediate coupling regime where $U \lesssim t$. It was observed in a previous work that in this regime the mean field approximation is quite reliable for this class of systems [7].

We decouple the Hamiltonian using the unrestricted Hartree–Fock approximation (HFA),

$$Un_{i,\uparrow}n_{i,\downarrow} \to U\langle n_{i,\uparrow}\rangle n_{i,\downarrow} + Un_{i,\uparrow}\langle n_{i,\downarrow}\rangle - U\langle n_{i,\uparrow}\rangle\langle n_{i,\downarrow}\rangle, \quad (2)$$

where $\langle \cdots \rangle$ denotes the expectation value calculated with respect to the ground state. Now the Hamiltonian can be divided into two parts for the two types of spins, i.e. $H = H_\uparrow + H_\downarrow$. In an unrestricted Hartree–Fock approximation, one determines the distribution of the $n_{i,\sigma}$ by diagonalizing $H_\uparrow$ and $H_\downarrow$ in a self-consistent manner. The ground state is constructed by filling the energy levels from both the up- and the down-spin bands up to the Fermi level.

In this paper, we have presented the results for two different types of superlattice structures as shown in figure 1. For the first one the size of the unit cell is two and for the second one it is three. We have taken two types of sites with on-site correlation parameters $U = 1$ and $U = 0$ respectively. We have set $t = 1$. We have studied the superlattices for various values of N. Since our aim is to compare the effects of the electric field on different superlattice structures of small size, we have presented here the results for the cases with $N = 60$ and 120 only. Comparing the results for these two system sizes one can also obtain an idea of what happens in the infinite limit.

To study the effect of the electric field on the metallic/insulating behavior of the ground state, we performed a systematic study of the charge gap (Δ) at the Fermi level of the system containing n electrons,

$$\Delta = E_{n+1} + E_{n-1} - 2E_n, \quad (3)$$

where E_n is the ground state energy of an n electron system. We have also studied the charge density wave (CDW) structure factor

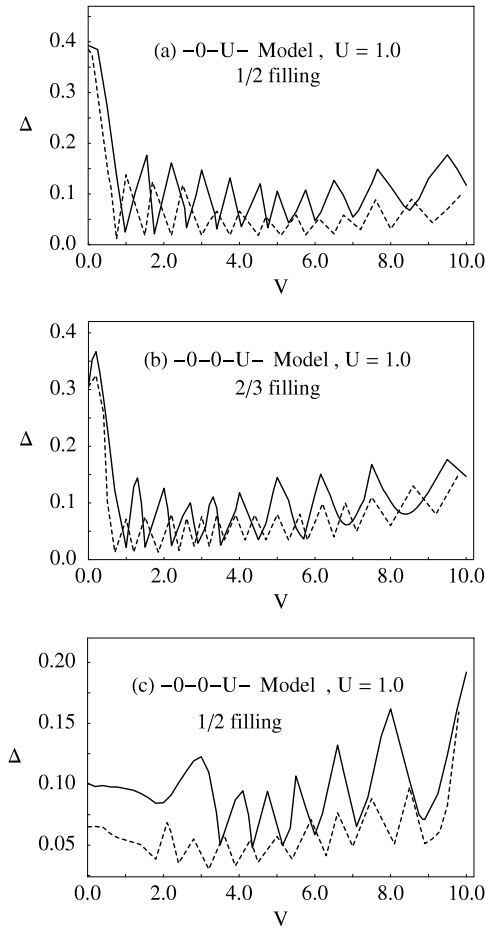$$C(q) = \frac{1}{N}\sum_{i,j} e^{iq(r_i-r_j)}(n_i - \rho)(n_j - \rho), \quad (4)$$
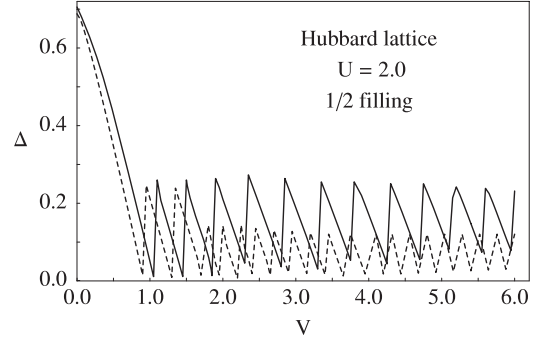
Figure 2. Variation of the charge gap (Δ) at the Fermi level for the homogeneous Hubbard chain at half-filling with the applied voltage (V). The solid line corresponds to $N = 60$, while the dotted line shows the case of $N = 120$.

where ρ is the average particle density on the superlattice, r_p denotes the position of the pth site and q is the wavevector. These two quantities enable us to capture the competition between the electric field and the correlation parameter in determining the charge modulation along the superlattice.

3. Results of HFA calculations

It is well known that in the absence of an electric field a homogeneous Hubbard chain is an antiferromagnetically ordered system with a finite charge gap at half-filling [17, 18]. Figure 2 shows the variation of the charge gap with the electric field for a half-filled homogeneous Hubbard chain. It is clear from the diagram that the charge gap goes through a number of maxima and minima with increasing electric field. As N increases the minima shift towards lower values of V. The nature of variation of the charge gap is in good qualitative agreement with the previous density matrix renormalization group (DMRG) results [15].

Now we discuss the results for the –0–U– superlattice structure. At half-filling the system is a CDW insulator with $q = \pi$ in the absence of electric field [5, 7] and the charge gap is finite ($V = 0$ case in figure 3(a)). As we turn on and gradually increase the electric field, the charge gap passes through a number of maxima and minima. For $N = 60$ and 120 the variation of the charge gap are shown in figure 3(a). The type of oscillation of the charge gap with electric field is quite similar to that observed in the homogeneous system (figure 2). These oscillations are observable only in the finite sized systems and are crucially controlled by the interplay of the Hubbard interaction and the spatial gradient of the external bias. In the absence of electric field, the CDW phase (with $q = \pi$) at half-filling has the tendency to form 'doublons' ($\uparrow\downarrow$) at the sites with $U = 0$, while the sites with $U > 0$ tend to depopulate. When the electric field is increased the electrons are pushed back near one end of the lattice. This leads to population of some sites with $U > 0$, leading to the breakdown of the $q = \pi$ CDW phase. Such a crossover from the CDW phase is marked by the first minimum in the charge gap. Subsequent increase in the electric field results in gradual accumulation of electrons in one half of the
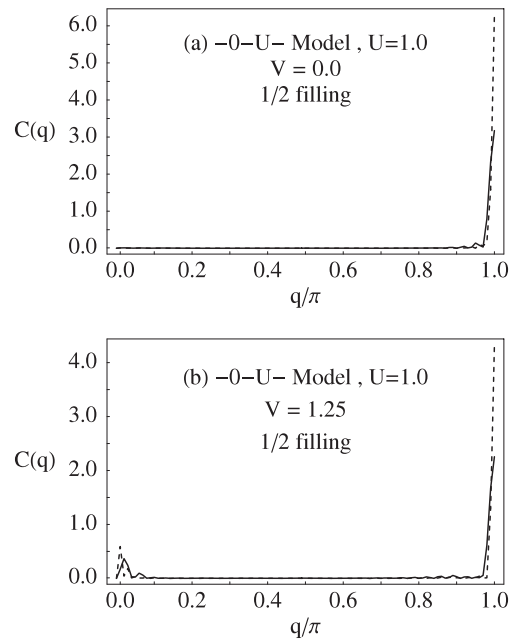
Figure 4. Charge density structure factor $C(q)$ for the half-filled –0–U– superlattice systems; (a) for $V = 0.0$ and (b) for $V = 1.25$ respectively. The solid line corresponds to $N = 60$, while the dotted line represents the case of $N = 120$.

Figure 3. Variations of the charge gap (Δ) at the Fermi level of the superlattice systems with the applied voltage (V); (a) for a –0–U– superlattice at half filling, (b) for a –0–0–U– superlattice at $\frac{2}{3}$ filling and (c) for a –0–0–U– superlattice at half filling respectively. The solid line corresponds to $N = 60$, while the dotted line shows the case of $N = 120$.

superlattice. Because of the competition between the Coulomb correlation energy and the electric field term, the aforesaid process of piling up of electrons takes place only after finite increments of electric field in a finite sized system. This results in the oscillation in the charge gap.

Next we study the CDW structure factor of this model. Generally speaking, from the mean field point of view, all sites with the same value of U in a superlattice are of same status. So a peak depending on the periodicity of the structure of the superlattice appears in the charge density structure factor. Our method also detects other peaks in the $C(q)$ that depend on the specific values of the density (i.e. the position of the peak depends on the Fermi wavevector k_F). As the system size N increases, the peak due to the structural periodicity of the lattice becomes larger compared to the other peaks. Under periodic boundary conditions or in the limit of $N \to \infty$, only the peak due to the structural modulation survives and the other peaks disappear.

Referring to the specific case of the –0–U– superlattice at half-filling, there is a sharp peak in $C(q)$ at $q \simeq \pi$ in the absence of electric field (figure 4(a)). Incidentally, in this case

the peak due to the periodicity of the lattice structure and the $2k_F$ peak both occur at $q \simeq \pi$. As the electric field is increased, after a critical value of the same, a peak at $q \simeq 0$ is seen (see figure 4(b)). This is due to accumulation of the charges near one side of the chain. At this value of the electric field, the peak at $q \simeq \pi$ starts to get diminished. For larger electric field, the peak at $q \simeq 0$ becomes larger at the cost of the peak at $q \simeq \pi$. In figure 5(a) the variations of the magnitudes of the peaks at $q \simeq 0$ and $q \simeq \pi$ are shown. It clearly shows that the value of the electric field at which the $q \simeq 0$ peak becomes significant is as same as the value of the electric field where the first minimum of the charge gap oscillation occurs (see figure 3(a)). So it is clear that at this value of the electric field charge accumulation at one side of the chain begins to dominate and the charge ordering tends to get destroyed. This point can be taken as a transition point, though on either side of it the system remains insulating. By observing the increase in height of the peak at $q \simeq 0$, one can easily understand how the charge accumulation on one side of the chain grows with electric field.

In figure 3(b) we present the variation of the charge gap with the electric field for the other system, the –0–0–U– superlattice at two-thirds filling. At zero electric field, the electrons try to accumulate at the sites with zero Hubbard interaction as this minimizes the energy. As a result, the system is a charge ordered insulator with a finite charge gap. A sharp peak of $C(q)$ at $q \simeq \frac{2\pi}{3}$ is obtained. Here also the density dependent $2k_F$ peak and the peak due to the structural periodicity of the lattice occur at the same q ($\simeq \frac{2\pi}{3}$). On application of the electric field, the charge gap initially increases and then gradually falls. Subsequent oscillations are observed as in the previous case of the –0–U– model.
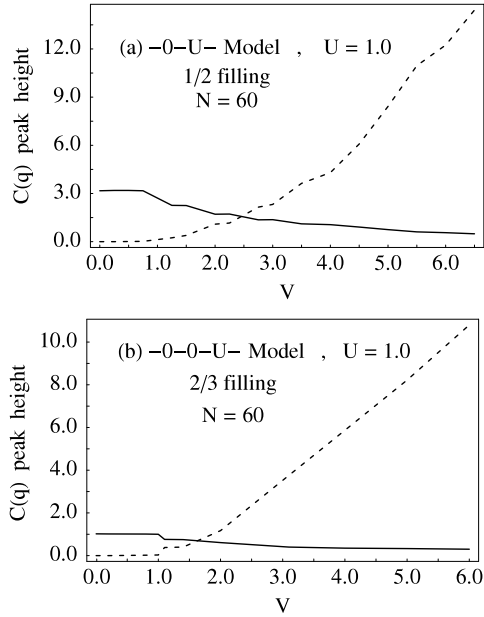
Figure 5. Variations of the height of the peaks in $C(q)$ for the superlattice systems with the applied voltage (V); the dashed line is for the peak at $q \simeq 0$, while the solid line is for the peak at $q \simeq \pi$ and $q \simeq \frac{2\pi}{3}$ in (a) the –0–U– superlattice at half filling and (b) the –0–0–U– superlattice at two-thirds filling respectively.

Figure 6. Variations of the charge gap (Δ) at the Fermi level for the quarter-filled superlattice systems with the applied voltage (V): (a) for the –0–U– superlattice and (b) for the –0–0–U– superlattice respectively. The solid line corresponds to $N = 60$, while the dotted line shows the case of $N = 120$.

The initial increase in the charge gap for small values of the electric field can be understood in the following way. In a particular cell of this –0–0–U– superlattice at two-thirds filling, the two sites on the left (with $U = 0$) are preferred by the electrons in the absence of electric field; they tend to be doubly occupied, keeping the other site empty. In this situation a charge density wave is formed in the chain. For nonzero electric field, there is a positive gradient of the site potentials towards the right (see figure 1). Then the distribution of the site potentials in a unit cell of the superlattice is in unison with the distribution of the correlation parameter. This phenomenon reinforces the aforesaid charge ordering for small values of the electric field. So an increase in the value of the charge gap is observed. For larger electric field, however, the spatial gradient of the site potentials becomes so large that a global shift of the charges towards the left is preferred in the chain and the charge ordering is destroyed. Also for the –0–U– model a trace of such feature is observed for low electric field. There is a change in the slope of the charge gap as a function of the applied voltage, for a low value of the voltage (see figure 3(a)). Since in this case the unit cell contains only two sites, the feature only shows up weakly. In contrast, we have noted that for the –U–0–0– model and –U–0– model this type of enhancement of charge ordering for small values of the electric field is absent. In these cases, on application of the electric field the charge gaps initially fall and then subsequent oscillations are observed.

Figure 5(b) shows the variation of the heights of the peaks of $C(q)$ with external bias for the –0–0–U– model; the type of variation is quite similar to the previous case of the –0–U– model. The peak at $q \simeq \frac{2\pi}{3}$ starts to fall and a peak at $q \simeq 0$ appears at a critical value of the electric field. This
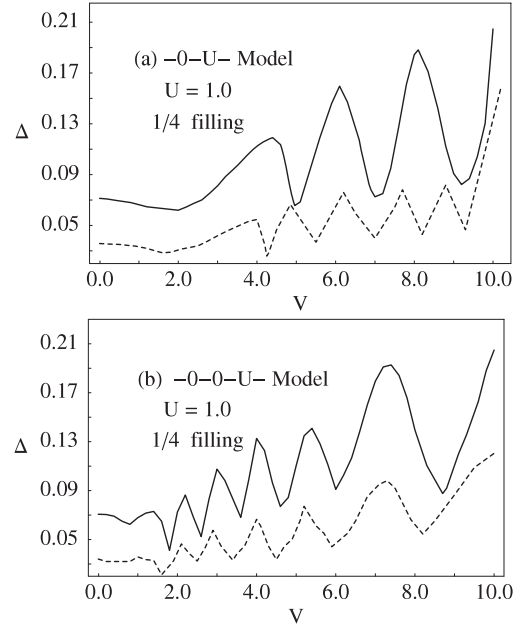
critical value again matches with the value of the electric field at which the first minimum of the charge gap oscillation occurs in figure 3(b). So in this case also it makes a transition from a CDW phase to a phase where electrons pile up at one end.

We have shown the variation of the charge gap for the –0–0–U– superlattice at half-filling in figure 3(c) for the sake of comparison with the other half-filled cases shown in figures 2 and 3(a). Here at $V = 0$ the gap diminishes with larger values of N, indicating a metallic behavior at the thermodynamic limit. An increase in V drives the system ultimately to an insulating one.

We have also studied the quarter-filled cases for our superlattice models. Figures 6(a) and (b) show the charge gap oscillations in the –0–U– and –0–0–U– models respectively. Both the systems are metallic in the absence of the electric field; the charge gap $\Delta \sim \frac{1}{N}$, N being the system size. With the increase of electric field the charge gap oscillates between a number of maxima and minima, and then increases monotonically, indicating an insulating phase.

In figure 7 we plot the $C(q)$ for both types of superlattice at quarter-filling in the absence of the electric field. For the –0–U– model (figure 7(a)), we see a dominant peak at $q = \pi$, which is due to the structural periodicity of the lattice. Apart from this, a $2k_F$ peak appears at $q \simeq \frac{\pi}{2}$. Also, a few other wiggles due to various possible short length scale density modulations are observed. For the –0–0–U– model (figure 7(b)) also, the dominant peak is due to the lattice structure and it occurs at $q = \frac{2\pi}{3}$. Here also other wiggles due to different possible density modulations are obtained along with the $2k_F$ peak ($q \simeq \frac{\pi}{2}$).

It can be seen explicitly, in the limit $U = 0$, that the position of the $2k_F$ peak in finite chains is shifted from the
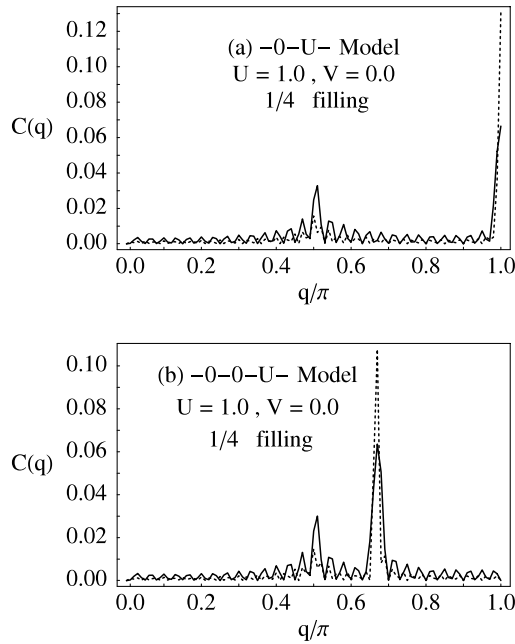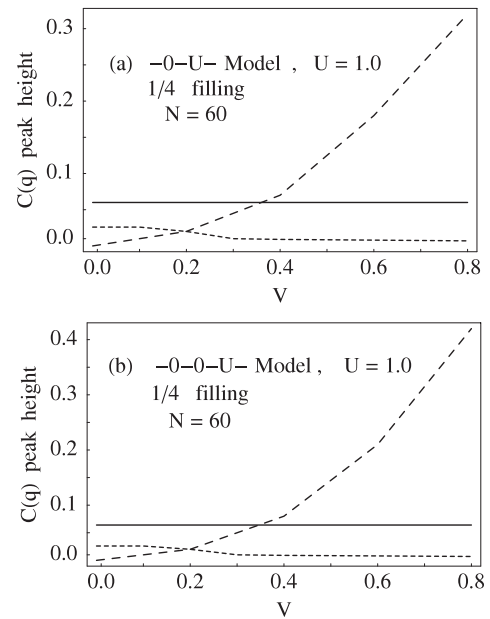
Figure 7. Charge density structure factor $C(q)$ for the quarter-filled superlattice systems at zero electric field: (a) for the –0–U– superlattice and (b) for the –0–0–U– superlattice respectively. The solid line corresponds to $N = 60$, while the dotted line shows the case of $N = 120$.

Figure 8. Variations of the height of peaks in $C(q)$ for the quarter-filled superlattice systems with the applied voltage (V); the dashed line is for the peak at $q \simeq 0$, the short dashed line is for the peak at $q \simeq \frac{\pi}{2}$ ($2k_F$) and the solid line is for the peak due to the structure (a) for the –0–U– superlattice and (b) for the –0–0–U– superlattice respectively.

expected position $q = 2k_F = n\pi/(N+1)$ (n being the number of occupied single particle levels) by an amount $\sim \frac{1}{N}$. As the system size N increases, they approach the actual $2k_F$ value. On the other hand, the peak heights fall as $\frac{1}{N}$. So in the large N limit (and also under periodic boundary conditions) the $2k_F$ peaks are not detectable.

As the electric field is turned on and increased, a peak at $q \simeq 0$ appears for both the models at quarter-filling. The peak due to the structural periodicity and the $2k_F$ peak (also the wiggles in $C(q)$) fall off; the rate of fall is much slower for the structural periodicity peak. These show the gradual accumulation of the charges near one side of the chain. In figure 8 variations of the heights of the peaks in the $C(q)$ with the external bias are shown. It clearly shows how charge accumulation at one side of the chain increases with electric field.

4. Conclusion

In this work, we have studied the one-dimensional Hubbard superlattices with different types of unit cells in the presence of electric field. The single-orbital nearest-neighbor tight-binding model has been used. We have maintained fixed system sizes ($N = 60$ and 120) for the purpose of comparison of these models. The charge gap and the CDW structure factor of the systems are studied under the Hartree–Fock approximation in the presence of electric field. To check the reliability of the Hartree–Fock approximation results, we compared our results for the homogeneous Hubbard model with a previous DMRG calculation [15] and found reasonable qualitative agreement. Oscillations in charge gap obtained in the superlattice systems

are rather similar to those observed in the homogeneous Hubbard chains, showing the signature of finite size. Variations of the heights of different peaks of $C(q)$ with the applied electric field give an idea about the distribution of electrons on the lattice. We found that the $2k_F$ peaks of $C(q)$ arise for finite sized systems only. On application of the electric field a peak at $q \simeq 0$ appears at a critical value of the field and then increases in height; other peaks fall gradually, indicating suppression of the ordering due to the Hubbard correlation on the superlattice. The rate of fall of the peak corresponding to the structural periodicity is much slower than the $2k_F$ peak. At the critical value of the electric field where the peak at $q \simeq 0$ appears in $C(q)$, the first minimum of the charge gap is observed for the systems which were initially charge ordered. The present mean field approximation is capable of detecting the variations of the charge structure with the electric field. One can also use other methods to study these features. We have presented here only two types of superlattices with a few different fillings. For other superlattice structures and for other fillings the effect of the electric field may also be explored. The superlattices at finite temperatures may reveal some interesting features on application of the electric field.

Acknowledgment

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