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Reduction of the charge-density-wave amplitude in a strongly correlated system

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Abstract. The competition between strong electronic correlations and charge ordering due to an external potential are studied in the infinite-U Hubbard model by means of the slave-boson technique. The quasi-particle screening of the external potential produces a reduction of the charge-density-wave amplitude with respect to the non-interacting (i.e. $U = 0$) case. The mechanism becomes more and more effective as the number of electrons per site is increased towards unity.

1. Introduction

The investigation of the competition between charge ordering and strong on-site electronic correlations is usually complicated by the fact that in most physical systems the mechanism that leads to the appearance of a charge-density wave (CDW) is the electron–electron interaction, and/or the coupling of electronic density to the lattice. The technical task of a proper treatment of such interaction terms in the intermediate- to strong-coupling regime, which is of relevance in the case of competing strong correlations and charge ordering [1], makes the results inconclusive.

There are however systems in which the driving forces for CDW formation are provided by the chemical environment. Such is for instance the case for π-chains on the Si(111) and C(111) reconstructed surfaces [2], where a charge modulation is produced by the external (crystal) field imposed on the surface by the bulk. In the presence of an efficient screening mechanism associated with a corresponding modulation of the substrate, the intra-atomic interaction among the π-electrons is the largest and most relevant contribution to the Coulombic interaction. This term may be treated in the Hartree–Fock approximation in the weak-coupling limit, and by means of the Kotliar–Ruckenstein slave bosons [3] in the intermediate- to strong-coupling regime. In this paper I address the issue of the competition between such an *external* CDW and an infinitely strong intra-atomic repulsion, within the framework of the infinite-U Hubbard model. This limiting case represents a simplification from the point of view of the slave-boson technique, since a single slave-boson operator is required. The calculations become thus more transparent, and it is possible to provide a simple quasi-particle interpretation of the properties of the system.

For the sake of definiteness, I consider the case of one spatial dimension, which is suitable for the quasi-one-dimensional system of loosely bound π-chains discussed above. However, due to the mean-field character of the forthcoming analysis, the results presented below are quite general, at least as far as ground-state properties are concerned, and the

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method described in the following may be extended to higher dimensions, where more complex structures of *external* CDW may be investigated [4].

It should be pointed out that in one dimension approaches alternative to the one presented below are possible for investigating the effect of an external potential on a system of interacting electrons [5–7]. There are, however, good reasons to adopt a complementary point of view. Indeed, the exact solutions available for a few one-dimensional models are often *opaque* [6], so extracting physical information requires further elaboration which mostly relies on quantum-field theory and perturbation theory. The latter is very likely to be not convergent in the strong-coupling limit $U \to \infty$ considered in this paper, in which case one has to go back to the exact solution (when available) and *argue* that fixed-point properties are the same at all couplings [8, 9]. Moreover the instability of the fluid state is usually seen as the evolution of the renormalized couplings to strong coupling under the renormalization group, while a clear description of broken-symmetry phases is not achieved.

On the other hand, slave bosons are known not only to provide an alternative bosonization scheme [10], but also to give a qualitatively good quasi-particle description of the infinite-U Hubbard model. In this limiting case, the velocity of spin excitations is indeed zero [8], and the system behaves as a collection of non-interacting spinless fermions at all fillings (the hard-core constraint being imposed by the Pauli principle), with the resulting Fermi velocity determining the behaviour of the charge excitations. Such a scenario is qualitatively well reproduced within the slave-boson approach [11]. Last but not least, the slave-boson technique is not specific to one-dimensional systems, and can be directly extended to higher dimensions.

Indeed, as will become clearer in the following, nothing specific to one-dimensional systems is discussed in the present paper, where the attention is focused on generic features, namely on the quasi-particle screening of an external potential in a strongly correlated system. For the same reason, peculiarities such as the $2k_F$-instabilities are not taken into account. The systems which are discussed in the present paper are those in which the structure of the charge modulation is provided by the external potential.

The plan of the paper is as follows. In section 2, I introduce the Hubbard model for a system with an *external* CDW, and describe the slave-boson (SB) technique which is suited for dealing with the limit of an infinitely large intra-atomic repulsion. The conditions for a CDW to exist and the mean-field ground-state properties of the system are analysed in section 3. Concluding remarks are found in section 4.

2. The model

I consider the Hubbard model in an external crystal field defined by the Hamiltonian

$$\tilde{\mathcal{H}} = -t \sum_{n,\sigma} (\tilde{f}^{\dagger}_{n,\sigma} \tilde{f}_{n+1,\sigma} + \text{HC}) - \sum_{n,\sigma} (I \mathrm{e}^{\mathrm{i}n\pi} + \mu) \tilde{f}^{\dagger}_{n,\sigma} \tilde{f}_{n,\sigma} + U \sum_{n} \tilde{f}^{\dagger}_{n\uparrow} \tilde{f}_{n\uparrow} \tilde{f}^{\dagger}_{n\downarrow} \tilde{f}_{n\downarrow}$$

where $\tilde{f}^{\dagger}_{n,\sigma}$, $\tilde{f}_{n,\sigma}$ are the fermion operators acting on site n in the Wannier representation, t is the nearest-neighbour hopping parameter, I is the amplitude of a staggered potential, which is produced by the external (crystal) field, μ is the chemical potential, and U is the on-site Coulombic repulsion. The limit $U \to \infty$ is usually treated within the SB approach by introducing additional degrees of freedom to keep track of the empty sites [12]. The fermion operators are decoupled as products of pseudo-fermion and boson operators $\tilde{f}^{\dagger}_{n,\sigma} \to f^{\dagger}_{n,\sigma} b_n$,

so the constraint of no double occupancy

$$\sum_{\sigma} \tilde{f}^{\dagger}_{n,\sigma} \tilde{f}_{n,\sigma} \leqslant 1$$

reads as a completeness relation

$$\sum_{\sigma} f^{\dagger}_{n,\sigma} f_{n,\sigma} + b^{\dagger}_{n} b_{n} = 1$$

in the new Fock space. Indeed, empty sites are now regarded as sites occupied by bosons. The pseudo-fermions play the role of quasi-particles with weak residual interaction. The constraints have to be imposed on the original Hamiltonian by site-dependent Lagrange multipliers λ_n, so the full SB Hamiltonian reads

$$\mathcal{H} = -t \sum_{n,\sigma} (b^{\dagger}_{n+1} b_n f^{\dagger}_{n,\sigma} f_{n+1,\sigma} + \mathrm{HC}) - \sum_{n,\sigma} (I \mathrm{e}^{\mathrm{i}n\pi} + \mu) f^{\dagger}_{n,\sigma} f_{n,\sigma} + \sum_{n} \lambda_n \left(\sum_{\sigma} f^{\dagger}_{n,\sigma} f_{n,\sigma} + b^{\dagger}_{n} b_n - 1 \right).$$

The mean-field Hamiltonian in the staggered external potential depends on the expectation values of the SB operators, and the Lagrange multipliers depend on the two inequivalent sites of the lattice, $\langle b_n \rangle = b_{\mathrm{A}}, b_{\mathrm{B}}$, $\langle \lambda_n \rangle = \lambda_{\mathrm{A}}, \lambda_{\mathrm{B}}$, where A and B label the two inequivalent sublattices, of even and odd site indices respectively. It should be observed that in the case of nearest-neighbour hopping considered here, the hopping term always involves sites belonging to different sublattices, so all of the sites are equivalent as far as hopping is concerned, and only the external potential explicitly breaks the translational invariance of the lattice. This would no longer be true should next-to-nearest-neighbour hopping be included. In the present case the diagonalization of the mean-field Hamiltonian may be performed in a simple way by explicitly separating the A and B sublattices:

$$\mathcal{H}_{mf} = -t b_{\mathrm{A}} b_{\mathrm{B}} \sum_{\substack{j \in A, \ell = \pm 1 \\ \sigma}} (f^{\dagger}_{j,\sigma} f_{j+\ell,\sigma} + f^{\dagger}_{j+\ell,\sigma} f_{j,\sigma}) + \sum_{\substack{j \in A \\ \sigma}} \left[(\lambda_{\mathrm{A}} - I - \mu) f^{\dagger}_{j,\sigma} f_{j,\sigma} + (\lambda_{\mathrm{B}} + I - \mu) f^{\dagger}_{j+1,\sigma} f_{j+1,\sigma} \right] + \frac{N_s}{2} \left[\lambda_{\mathrm{A}} (b^2_{\mathrm{A}} - 1) + \lambda_{\mathrm{B}} (b^2_{\mathrm{B}} - 1) \right]$$

where N_s is the number of lattice sites. The above Hamiltonian is immediately transformed to k-space with respect to the A sublattice (i.e. with respect to the index j), the vector k thus belonging to the Brillouin zone of the A sublattice, i.e. the reduced Brillouin zone of the original lattice. The transformation rules of the pseudo-fermion operators are defined as

$$f_{j,\sigma} = \sqrt{2/N_s} \sum_{k} A_{k,\sigma} \mathrm{e}^{-\mathrm{i}kj}$$

$$f_{j+\ell,\sigma} = \sqrt{2/N_s} \sum_{k} B_{k,\sigma} \mathrm{e}^{-\mathrm{i}k(j+\ell)}$$

for $j \in A$, $\ell = \pm 1$ [13]. The operators $A^{\dagger}_{k,\sigma}$ and $B^{\dagger}_{k,\sigma}$ create a Bloch wave of A and B pseudo-electrons respectively. The two Bloch states are mixed by the hopping term, which transforms A electrons into B electrons and vice versa. The mean-field Hamiltonian in the k-space representation is diagonalized by a canonical Bogoliubov transformation [14] to yield the quasi-particle spectrum

$$E^{\pm}_{k} = \lambda_0 - \mu \pm \sqrt{(I - \lambda_c)^2 + 4t^2 b^2_{\mathrm{A}} b^2_{\mathrm{B}} \cos^2 k} \tag{1}$$

where

$$\lambda_0 = \frac{1}{2}(\lambda_A + \lambda_B) \qquad \lambda_c = \frac{1}{2}(\lambda_A - \lambda_B)$$

and $k \in [-\pi/2, \pi/2]$, the lattice spacing being taken as the unit length. At this point it is worth noting that the above spectrum is easily generalized to the case of a cubic lattice in d dimensions in an external potential of wave-vector $(\pi, \ldots, \pi)$, by taking

$$\cos k \to \sum_{\alpha=1}^{\alpha=d} \cos k_\alpha .$$

As will become clearer in the following, the parameter λ_c describes the quasi-particle screening of the external potential I, which is reduced to $\tilde{I} = I - \lambda_c$. Besides a trivial rescaling of the chemical potential $\tilde{\mu} = \mu - \lambda_0$, the effect of strong correlations is also seen in the reduction of the hopping parameter $\tilde{t} = t b_A b_B$. Once these renormalizations are taken into account, the spectrum (1) again takes on the formal aspect of the spectrum of a non-interacting system in an external staggered potential; in the interacting case, however, the band-width and the amplitude of the external potential are to be fixed self-consistently. This formal analogy allows for an immediate comparison between the $U = \infty$ and $U = 0$ limits.

3. Mean-field results

The mean-field Hamiltonian in the quasi-particle representation reads

$$\mathcal{H}_{mf} = \sum_{k,\sigma} (E_k^+ \xi_{k,\sigma}^\dagger \xi_{k,\sigma} + E_k^- \eta_{k,\sigma}^\dagger \eta_{k,\sigma}) + \frac{N_s}{2}\left[\lambda_0(b_A^2 + b_B^2 - 2) + \lambda_c(b_A^2 - b_B^2)\right] \tag{2}$$

where

$$\xi_{k,\sigma} = u_k A_{k,\sigma} + v_k B_{k,\sigma}$$
$$\eta_{k,\sigma} = v_k A_{k,\sigma} - u_k B_{k,\sigma}$$

are the quasi-particle operators for the upper and lower bands respectively, and

$$u_k^2 = \frac{1}{2}\left[1 - \frac{I - \lambda_c}{\sqrt{(I - \lambda_c)^2 + 4t^2 b_A^2 b_B^2 \cos^2 k}}\right]$$
$$v_k^2 = \frac{1}{2}\left[1 + \frac{I - \lambda_c}{\sqrt{(I - \lambda_c)^2 + 4t^2 b_A^2 b_B^2 \cos^2 k}}\right]$$

are the weights of the A and B pseudo-electrons in the quasi-particle wave-functions. For $I - \lambda_c \to 0$ the quasi-particles are equal admixtures of A and B pseudo-electrons, whereas in the opposite limit $I - \lambda_c \gg 2t b_A b_B$ the lower band has mainly A character and the upper band has mainly B character.

The mean-field parameters $b_A, b_B, \lambda_A, \lambda_B$ are determined by solving self-consistency equations of the form $\partial \langle \mathcal{H}_{mf} \rangle = 0$, where the derivatives are taken with respect to the mean-field parameters and $\langle \cdots \rangle$ is the average in the ground state [15]. The chemical potential μ is chosen to fix the average number of electrons per unit cell $n = 1 - \delta$, where

δ is the hole doping with respect to half-filling. At $T = 0$ only the lowest band E_k^- is occupied for $n < 1$. The self-consistency equations are then

$$\begin{cases} n = 2N_s^{-1}\sum_k \Theta(E_k^-) \\ \frac{1}{2}(b_A^2 + b_B^2) = 1 - n \\ \frac{1}{2}(b_A^2 - b_B^2) = 2N_s^{-1}\sum_k R_k^{-1}(\lambda_c - I)\Theta(E_k^-) \\ \lambda_c = N_s^{-1}4t^2(b_A^2 - b_B^2)\sum_k R_k^{-1}\cos^2 k\ \Theta(E_k^-) \\ \lambda_0 = N_s^{-1}4t^2(b_A^2 + b_B^2)\sum_k R_k^{-1}\cos^2 k\ \Theta(E_k^-) \end{cases} \tag{3}$$

where a factor of 2 in the r.h.s. of each equation is due to the sum over the spin index σ, the sum over k is restricted to the reduced Brillouin zone of the original lattice, $\Theta(x) = 1$ for $x < 0$, and zero otherwise, is the zero-temperature limit of the Fermi function, and

$$R_k = \sqrt{(I - \lambda_c)^2 + 4t^2 b_A^2 b_B^2 \cos^2 k}.$$

To make the above equations more transparent, observe that the number of electrons on the two inequivalent sites may be written as $n_A = n + m$ and $n_B = n - m$ in terms of the average density n and the CDW amplitude m. Then, the local constraint imposes $b_A^2 = 1 - n_A$, $b_B^2 = 1 - n_B$, so $b_B^2 - b_A^2 = n_A - n_B = 2m$. The renormalization of the hopping parameter is given by

$$b_A b_B = \sqrt{(1-n)^2 - m^2} = \sqrt{\delta^2 - m^2}$$

whence it is evident that $m^2 \leqslant \delta^2$, i.e. the CDW amplitude may not increase beyond δ, double occupancy being forbidden. This, in turn, implies that the system cannot sustain a CDW at half-filling ($\delta = 0$), and a severe reduction of the CDW amplitude is expected for small δ. In terms of the new parameters the self-consistency equations are

$$\begin{cases} \delta = 1 - 2N_s^{-1}\sum_k \Theta(E_k^-) \\ m = 2N_s^{-1}\sum_k R_k^{-1}(I - \lambda_c)\Theta(E_k^-) \\ \lambda_c = N_s^{-1}8t^2 m\sum_k R_k^{-1}\cos^2 k\ \Theta(E_k^-) \\ \lambda_0 = \frac{\delta}{m}\lambda_c \end{cases} \tag{4}$$

with

$$R_k = \sqrt{(I - \lambda_c)^2 + 4t^2(\delta^2 - m^2)\cos^2 k}.$$

The above equations involve incomplete elliptic integrals, and may be investigated numerically. However, good insight into their physical content is gained by simplifying the calculations within logarithmic accuracy. Indeed, all of the functions appearing in (4) depend on $k \in [-\pi/2, \pi/2]$ only through $\cos k$ (or through $\sum_{\alpha=1}^{\alpha=d}\cos k_\alpha$ in d dimensions), so

$$N_s^{-1}\sum_k \varphi(\cos k) \equiv \frac{1}{2}\int \mathrm{d}\varepsilon\ \mathcal{N}(\varepsilon)\varphi(\varepsilon)$$

with

$$\mathcal{N}(\varepsilon) = 2N_s^{-1} \sum_k \delta(\varepsilon - \cos k).$$

I then assume $\mathcal{N}(\varepsilon)$ to be a uniform distribution in the interval $[0, 1]$ (or $[0, d]$ in d dimensions; see e.g. the first reference in [1]). The condition for particle number conservation immediately fixes the value of ε at the Fermi surface, $\varepsilon_F = \delta$. Moreover, since $\lambda_0 = (\delta/m)\lambda_c$, two independent equations remain:

$$\begin{cases} m = \dfrac{I - \lambda_c}{2t\sqrt{\delta^2 - m^2}} \displaystyle\int_\delta^1 \frac{\mathrm{d}\varepsilon}{\sqrt{z^2 + \varepsilon^2}} = z \ln \frac{1 + \sqrt{1 + z^2}}{\delta + \sqrt{\delta^2 + z^2}} \\ \lambda_c = \dfrac{2tm}{\sqrt{\delta^2 - m^2}} \displaystyle\int_\delta^1 \frac{\varepsilon^2}{\sqrt{z^2 + \varepsilon^2}}\, \mathrm{d}\varepsilon = \frac{tm}{\sqrt{\delta^2 - m^2}} \left[\sqrt{1 + z^2} - \delta\sqrt{\delta^2 + z^2} - mz \right] \end{cases} \tag{5}$$

where

$$z = (I - \lambda_c)/2t\sqrt{\delta^2 - m^2}.$$

Progress towards the solution of the above equations is made by observing that, for a given δ, m is a function of z, i.e. it depends on λ_c only through z. The limiting behaviours of $m(z)$ are

$$m(z) \sim 1 - \delta - (1 - \delta^3)/6z^2 \qquad \text{for } z \to \infty$$

and

$$m(z) \sim -z \ln \delta \qquad \text{for } z \to 0.$$

A sketch of $m(z)$ is given in figure 1. It must be pointed out that, due to the above-mentioned formal analogy between the $U = \infty$ and $U = 0$ quasi-particle spectra, the function $m(z)$ gives also the CDW amplitude m as a function of $z \equiv I/2t$ in the non-interacting case, so a comparison is immediately possible.

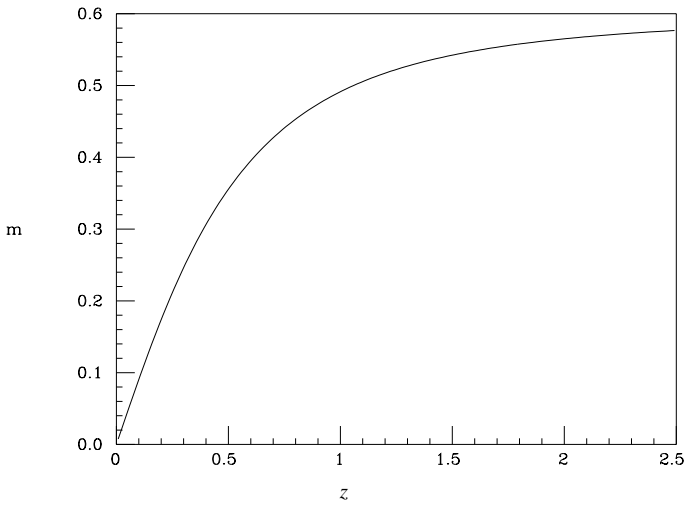

Figure 1. A sketch of the function $m(z)$, for $\delta = 0.4$.

At this point, self-consistency is simply imposed by (graphically) solving the two coupled equations

$$\begin{cases} \lambda_c = I - 2tz\sqrt{\delta^2 - m^2(z)} \\ \lambda_c = \dfrac{tm(z)}{\sqrt{\delta^2 - m^2(z)}}\left[\sqrt{1+z^2} - \delta\sqrt{\delta^2+z^2} - zm(z)\right] \end{cases} \tag{6}$$

where $m(z)$ is shorthand notation for the rightmost expression appearing in the first equation in (5). The system (6) is solved to yield the self-consistent values $\bar{z}$, $\bar{\lambda}_c$, whence $\bar{m} = m(\bar{z})$ and $\bar{\lambda}_0 = \delta\bar{\lambda}_c/\bar{m}$ are determined (see e.g. figures 2 and 3). Observe that the only dependence of the self-consistency equations on I is through the intercept of the curve represented by the first equation in (6), so this curve is rigidly shifted upwards as I is increased.

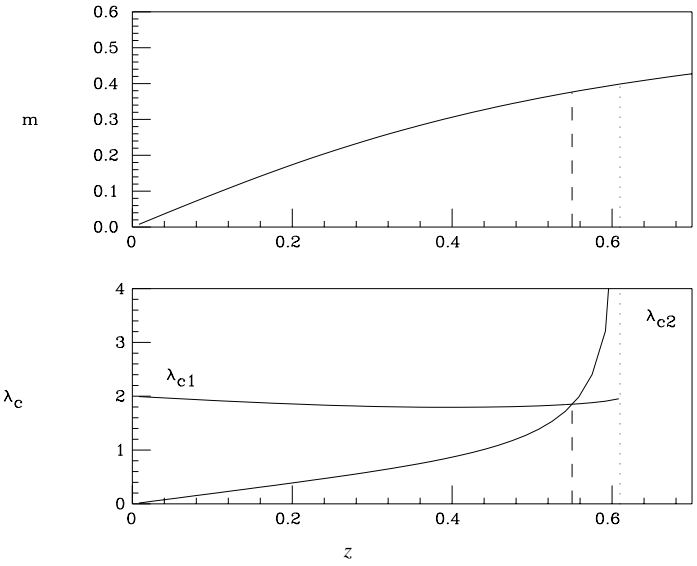

Figure 2. Top: a plot of the function $m(z)$ for $\delta = 0.4$. Bottom: a plot of the functions $\lambda_{c1}(z)$, the first equation in (6), and $\lambda_{c2}(z)$, the second equation in (6), for $\delta = 0.4$, $t = 1$, and $I = 2$. The value of I gives the intercept of the curve $\lambda_{c1}(z)$, which is rigidly shifted upwards (downwards) as I is increased (decreased). The dashed vertical lines mark the self-consistent values. The dotted vertical lines mark the point where $m = \delta$, which is a vertical asymptote for the curve $\lambda_{c2}(z)$.

In the last part of this section I want to discuss in detail the main properties of the solutions of (6), addressing in particular the issue of the quasi-particle screening of the CDW. Since $0 \leqslant n \leqslant 1$, two possibilities arise as I/t is increased.

(i) When $\frac{1}{2} < n \leqslant 1$, n_{A} saturates towards $n_{\mathrm{A},\infty} = 2n - 1 < 1$ and n_{B} saturates to $n_{\mathrm{B},\infty} = 1$, so the CDW amplitude saturates to $m_\infty \equiv \frac{1}{2}(n_{\mathrm{A},\infty} - n_{\mathrm{B},\infty}) = \delta$, i.e. the profile of the CDW is narrowed as $n \to 1$ ($\delta \to 0$), the quasi-particle screening becoming more and more effective (see below).

(ii) When $0 \leqslant n \leqslant \frac{1}{2}$, full saturation is possible, and $n_{\mathrm{A},\infty} = 0$, $n_{\mathrm{B},\infty} = 2n$, $m_\infty = n$, as in the non-interacting case.

The behaviour of the screening field λ_c confirms the above discussion. Indeed, the r.h.s. of the second equation in (6) diverges at $m = \delta$, so in the first case, when $\delta < 1 - \delta$,

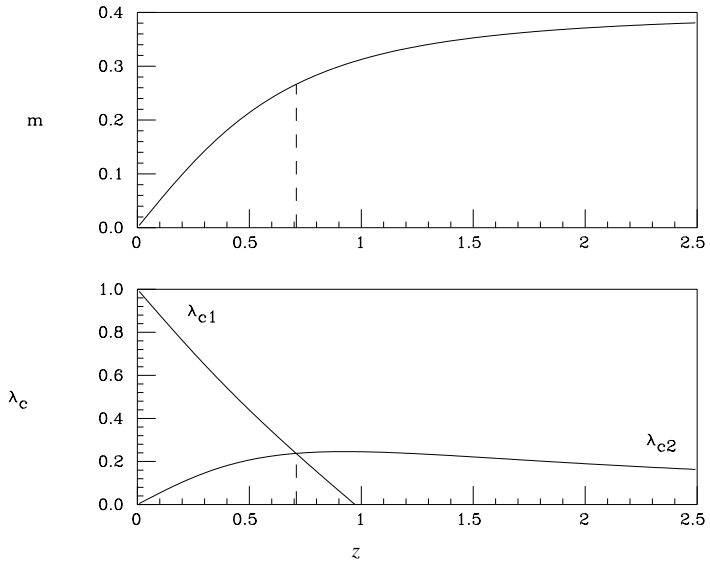

Figure 3. Top: a plot of the function $m(z)$ for $\delta = 0.6$. Bottom: a plot of the functions $\lambda_{c1}(z)$, the first equation in (6), and $\lambda_{c2}(z)$, the second equation in (6), for $\delta = 0.6$, $t = 1$, and $I = 1$. The value of I gives the intercept of the curve $\lambda_{c1}(z)$, which is rigidly shifted upwards (downwards) as I is increased (decreased). The dashed vertical lines mark the self-consistent values.

$\bar{z}$ stays finite as $I/t \to \infty$ since the equation

$$\bar{z} \ln \frac{1 + \sqrt{1 + \bar{z}^2}}{\delta + \sqrt{\delta^2 + \bar{z}^2}} = \delta \tag{7}$$

has a finite solution. Then, from the first equation in (6) it is seen that $\lambda_c \to I$ (complete screening, $\tilde{I} = I - \lambda_c \to 0$). Finally,

$$m \simeq \delta - (at/I)^2$$

where

$$a = (1 - \delta)[\sqrt{1 + \bar{z}^2} - \delta\sqrt{\delta^2 + \bar{z}^2} - \delta\bar{z}]/\sqrt{2\delta}$$

and $\bar{z}$ is the solution of (7). A typical representation for the case where $\delta < \frac{1}{2}$ is given in figure 2.

In the second case, $\delta > 1 - \delta$ ($> m$) and the r.h.s. of the second equation in (6) is not divergent, the point $m = \delta$ being unattainable. Then $\bar{z} \to \infty$ as $I/t \to \infty$ and

$$m \simeq 1 - \delta - (1 - \delta^3)/6\bar{z}^2 \to 1 - \delta.$$

Indeed, the second equation in (6) yields

$$\lambda_c/t \simeq 2(1 - \delta)(1 - \delta^3)/3\bar{z}\sqrt{2\delta - 1} \to 0$$

(the external potential is unscreened: $\tilde{I} \to I$), and from the first equation in (6)

$$\bar{z} \simeq I/2t\sqrt{2\delta - 1} \to \infty$$

which proves full self-consistency. A typical representation for the case where $\delta > \frac{1}{2}$ is given in figure 3. It should be observed that, in the present low-density regime, CDW formation may be favoured in the interacting system with respect to the non-interacting

case. This phenomenon can be understood by observing that, though the external potential I is essentially unscreened, the hopping parameter is still reduced in the interacting case, and saturates to

$$\tilde{t}_\infty = t\sqrt{2\delta - 1} < t$$

so the effective ratio $\tilde{I}/\tilde{t} > I/t$ corresponds to a larger CDW amplitude. The physical interpretation for this behaviour is that, in the low-density limit, the larger the CDW amplitude, the more the particles are kept apart from one another. The loss of kinetic energy in the CDW state is thus compensated in the interacting case by a gain in correlation energy, i.e. a reduction of the tendency towards double occupancy of the system.

4. Conclusions

In this paper I have investigated the competition between strong on-site correlations and CDW formation in systems where the charge ordering is driven by an external (crystal) field and long-range electron–electron interactions are screened due to the presence of a modulation in the chemical environment. In the extreme limit of an infinite on-site repulsion examined in this paper, a single slave boson was introduced, and a simple quasi-particle description of the system could be given. A formal analogy between the quasi-particle spectrum in the $U = \infty$ case and the band structure for a non-interacting system in the same external field was exploited to provide a clear scenario for CDW formation in such systems. Two situations may arise.

(i) In the high-density limit $\frac{1}{2} < n \leqslant 1$, the CDW amplitude is reduced with respect to that in the non-interacting case. The physical mechanism which leads to the suppression of the CDW amplitude is the quasi-particle screening of the external potential to prevent double occupancy. This screening mechanism becomes more and more effective as n increases towards unity. At $n = 1$, charge ordering is impossible, and the external field is completely screened.

(ii) In the low-density limit $n < \frac{1}{2}$, the screening mechanism is much weaker and the CDW amplitude saturates towards the free-particle value as the strength of the external potential is increased. In this regime, the CDW amplitude may be enhanced with respect to that in the non-interacting case due to a balance between the loss of kinetic energy and the gain in correlation energy. Indeed, as the CDW amplitude is increased, particles are kept further apart, and the tendency towards double occupancy is reduced.

The phase diagram in the I/t versus n plane corresponding to the above scenario is thus very simple. The system supports a CDW as soon as $I/t > 0$ and $n < 1$. This CDW phase is unique, and there is no further instability in the system as I/t is increased and/or n is decreased. When the properties of the CDW phase are compared to those of the corresponding non-interacting (i.e. $U = 0$) system, it is however clear that the line $n = \frac{1}{2}$ separates two regions in which the CDW amplitude in reduced ($n > \frac{1}{2}$) and in which it is enhanced ($n < \frac{1}{2}$) with respect to the case where $U = 0$. Only in this region is a full saturation of the CDW amplitude possible as I/t is increased.

The properties described so far refer to the CDW phase, and a comparison with previous results obtained in an investigation of the stability of the fluid state [6] in one-dimensional spinless systems is not straightforward. It must be assumed that the results obtained earlier suffer minor changes when spinning electrons are considered, and that the extrapolation $U \to \infty$ is harmless (see, e.g., [16]) regardless of the ratio I/t and of the filling δ.

It may, however, be observed that an external potential of the form

$$V \sim \int \mathrm{d}x \, \cos(\lambda x) n(x)$$

produces terms of the sine–Gordon type only when the periodicity is commensurate with the electronic density. In the present paper, $\lambda = \pi$, so such terms are produced at $n = 1/k$, $k = 1, 2, \ldots$, i.e. either for $n = 1$ (where no CDW exists), or for $n \leqslant \frac{1}{2}$ where the CDW amplitude is not reduced. Thus the most interesting region, $\frac{1}{2} < n < 1$, is beyond the range of applicability of a direct extension of those results. The reader interested in commensuration effects in one dimension may refer to [7] and references therein.

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[13] It should be noted that B_k is independent of $\ell = \pm 1$.
[14] See, e.g.,
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