The one-electron spectral-weight function of the half-filled ionic Hubbard model is calculated by means of Quantum Monte Carlo. A metallic regime occurs between two values of the coupling constant (Hubbard $U$) $U_1 < U_2$. The system is a band insulator below $U_1$, with a strong charge density wave corresponding to a large ionicity, and an increasingly antiferromagnetic (AF) insulator above $U_2$ evolving into a Mott insulator as $U \to \infty$. The intermediate regime, which is both AF and dimerized, is caused by a two-peak structure at $ka=0.5\pi$ (the Fermi surface). As $U$ increases both peaks approach each other, overlap, and separate again, the system becoming metallic in the overlap region. This behavior can be traced to a site-parity change of the ground state (GS), corresponding to a curve-crossing between two GS of different site parity.

PACS numbers: 71.30.+h,71.10. Pm, 77.80.-e

I. INTRODUCTION

In quasi-one dimensional materials like halogen-bridged transition metal chain complexes, conjugated polymers, organic charge transfer salts, or inorganic blue bronzes, the itinerancy of the electrons strongly competes with electron-electron and electron-phonon interactions which tend to localize the charge carriers by establishing commensurate spin or charge-density wave ground states (GS). At half filling band (BI) or Mott (MI) insulating phases are favored over the metallic state. Quantum phase transitions between the insulating phases are possible and the character of the electron excitation spectra reflect the properties of the different GS. A controversial issue is the nature of the BI-MI transition as well as whether or not only one critical point separates both insulating phases in purely electronic model Hamiltonians. Despite their importance in low dimensional materials, phonon
dynamical effects will be ignored in this paper which will be concerned with the so-called one dimensional (1D) ionic Hubbard model (IHM), just a Hubbard model with a staggered potential which displaces by $\Delta$ the energy levels of even and odd sites. It is described by the Hamiltonian

$$H = -t \sum_{<ij>_s} c_{is}^\dagger c_{js} + \frac{\Delta}{2} \sum_{is} (-1)^i n_{is} + U \sum_i \left( n_{is\uparrow} - \frac{1}{2} \right) \left( n_{is\downarrow} - \frac{1}{2} \right),$$

(1)

where electrons of spin $s = \pm \frac{1}{2}$ hop with amplitude $t$ between nearest-neighbor inequivalent sites of energy level $\pm \frac{1}{2} \Delta$ ($\Delta = 1$ in what follows). Electrons of opposite spin on the same site feel a repulsion $U$.

This model Hamiltonian, originally proposed by Nagaosa and later by Egami as a model ferroelectric, is ideal for studying the issue of quantum phase transitions in electron systems. On general grounds one expects a transition to occur from an ionic band insulator to a strongly-correlated Mott insulator as $U$ increases. Evidence for such a transition was found in exact-diagonalization calculations by Resta et al predicting a metallic point at a critical value $U = U_c$ separating both insulating phases. This transition is signaled by a polarization jump with a sign change associated with a site parity change of the GS. The same conclusion was supported by Gidopoulos et al who showed the reversal of site parity above to be of magnetic origin, thus leading to a vanishing of the spin gap, $\Delta_s = 0$. Likewise, Brune et al by means of the bosonization technique along with Lanczos and density matrix renormalization group (DMRG) calculations lent support to this picture.

On the other hand, Fabrizio et al shed new interest into the IHM in a field-theoretical bosonization analysis where they propose a new scenario for the intermediate region, $U \simeq \Delta$, between the BI and the MI. The model should instead exhibit two quantum phase transitions: one from a BI state to a long-range bond-ordered (BO) state predicted to be in the Ising universality class and a second one from the BO to the MI state predicted to be a Kosterlitz-Thouless transition. Such transitions to BO states have recently been found in 1D Hubbard models with extended interactions (U-V) by Nakamura. The BO state is a broken symmetry state in which the system becomes ferroelectric due strictly to electron-electron interactions even if all the atoms are at centers of inversion. This is also called the spontaneously dimerized insulating (SDI) phase, which, as argued by Fabrizio et al, implies a finite spin gap, $\Delta_s \succ 0$. Such a SDI phase has been observed numerically by Wilkens and Martin.
in a variational quantum Monte Carlo study. More precisely, they found one transition from the BI to the correlated SDI phase, but no second transition to the MI phase which is approached asymptotically by the SDI phase as \( U \to \infty \). Recent DMRG calculations lead to mutually conflicting results. Thus whereas Takada and Kido support the Resta et al. picture of a single first-order transition, Qin et al. support the Fabrizio et al. scenario of two second-order quantum phase transitions.

In this paper we present the one-electron spectral-weight function \( A(k,\omega) \) of the IHM. The calculation is done by means of a Quantum Monte Carlo (QMC) simulation in the grand canonical ensemble supplemented by an approximate effective action. Its eigenvalues and eigenvectors allow us to construct explicitly dynamic correlation functions in real time or frequency. This procedure leads to spectral functions with a reasonably high resolution. The calculation is performed at a relatively large inverse temperature, \( \beta t = 10 \) (\( t = 1 \) in what follows), which brings the system very close to its GS properties. Our calculated \( A(k,\omega) \) clearly shows metallic character (non-vanishing density of states in the gap) at \( ka = 0.5\pi \) \( (a = 1) \), between two critical \( U \) values instead of a single metallic point at the first threshold. Thus a double BI-M-MI smooth transition is predicted, the intermediate metallic regime at \( U \simeq 2\Delta \) being both antiferromagnetic (AF) and dimerized.

II. EFFECTIVE HAMILTONIAN AND CORRELATION FUNCTIONS

In our calculations, we use the QMC approach in the grand canonical ensemble, which has been explained in detail by Hirsch and White et al. As is well-known, the partition function is factorized into \( L \) time slices of extent \( \Delta \tau = \beta/L \). For Hubbard models, the interaction \( U \sum_i n_i \uparrow n_i \downarrow \) is transformed into a discrete Ising field, \( \sigma_{il} = \pm 1 \), which depends on lattice site \( i \) and imaginary time \( \tau = l\Delta \tau \) \( (l = 1, \ldots, L) \). The non-interacting Hamiltonian for a given Ising configuration (a definite allocation of +1 and −1 values for all the \( \sigma_{il} \) is) reads

\[
H(\tau) = \sum_{<ij> s} c_{is}^+ h_{ij}^s \{ \sigma_i(\tau) \} c_{js} \equiv H_i
\]

where

\[
h_{ij}^s \{ \sigma_i(\tau) \} = t_{ij} + \left( \Delta (-1)^i + \frac{U}{2} - \mu + \lambda \alpha \sigma_{il} \right) \delta_{ij}
\]
The first term on the rhs of Eq(3) is just the hopping term of the IHM, Eq(1). In the second term, \( \mu \) is the chemical potential, \( \alpha = \pm 1 \) for up/down electron spin, and \( \lambda \) is a non-linear function of \( U \) given by \( \cosh \lambda \Delta \tau = \exp (U \Delta \tau / 2) \). In the limit \( \Delta \tau \to 0 \) the partition function can be written as

\[
Z = \sum_{<\sigma>} \text{Tr} \Pi_t e^{-\Delta \tau H_t} = \sum_{<\sigma>} \text{Tr} e^{-\Delta \tau \sum_i H_i} = \sum_{<\sigma>} \text{Tr} e^{-\beta(K+V)}
\]

(4)

where \( \sum_{<\sigma>} \) means summing over the Ising configurations and \( \text{Tr} \) denotes taking the trace over the electron degrees of freedom. \( K \) is the \( \tau \)-independent part of \( H(\tau) \) and

\[
V = \frac{\lambda}{L} \sum_{i,l} \sigma_{il} (n_{i\uparrow} - n_{i\downarrow}) = \lambda \sum_i <\sigma_i> (n_{i\uparrow} - n_{i\downarrow})
\]

(5)

\( <\sigma_i> = (1/L) \sum_i \sigma_{il} \) being the average Ising spin at the \( i \)-th site. Therefore, \( H_{eff} = K + V \) is \( \tau \)-independent in the limit \( \Delta \tau \to 0 \). We adopt this effective \( \tau \)-independent Hamiltonian, for doing measurements even if the number of time slices used in the calculation is finite.

To minimize as much as possible size effects due to a finite \( L \), we shall increase \( L \) and seek for convergence. Needless to say, the update of the Ising field is done following the standard procedure of, say, Ref 15.

The corresponding Hamiltonian matrix for each spin \( s \) (Eq(3) with \( <\sigma> \) instead of \( <\sigma_{il}> \)) is now diagonalized and, in terms of its eigenvalues \( \varepsilon_{\mu s} \) and eigenvectors \( |\mu s> \), we can construct correlation functions in real time or frequency. For instance

\[
G_{ij}^s(\omega) = \sum_\mu <i|\mu s> \left\{ \frac{1 - f_{\mu s}}{\omega - \varepsilon_{\mu s} + i\eta} + \frac{f_{\mu s}}{\omega - \varepsilon_{\mu s} - i\eta} \right\} <\mu s | j> = G_{ij}^s(\omega) + G_{ij}^{s<}(\omega)
\]

(6)

for the causal Green’s functions and likewise for other quantities. As customary, \( f_{\mu s} = (e^{\beta \varepsilon_{\mu s}} + 1)^{-1} \) is the Fermi-Dirac distribution and \( \eta \) a vanishingly small imaginary part. All these quantities must now be averaged over the accepted Ising configurations to obtain the final result. It is just in this averaging process where the correlation effects are restored. Since the final result is translationally invariant, one can Fourier transform and find the spectral-weight function (SWF)

\[
A_{ks}(\omega) = -\frac{1}{\pi} \text{Im} \left\{ G_{ks}^>(\omega) - G_{ks}^{s<}(\omega) \right\},
\]

(7)

and the DOS

\[
N_s(\omega) = \frac{1}{N} \sum_{k'} A_{ks}(\omega)
\]

(8)
which can also be obtained from (6) as $(1/N) \sum_i N_i(\omega)$, $N_i(\omega)$ being the corresponding imaginary part of $G_{ii}^\ast(\omega)$. For our case of the IHM, this last route allows to calculate the partial DOS for even/odd atoms by simply restricting the sum over even/odd sites. As noticed earlier, this building procedure leads to a good resolution of spectral features.

III. DOUBLE INSULATOR-METAL-INSULATOR TRANSITION

We characterize the system by its one-electron SWF, $A_k(\omega)$, along with the charge and spin structure factors, $c_k$ and $s_k$, defined as the Fourier transform of the static charge and spin, respectively, correlation functions. These are given as usual by $c_{ij} = \langle q_i q_j \rangle$ and $s_{ij} = \langle s_{iz} s_{jz} \rangle$, $q_i = n_{i\uparrow} + n_{i\downarrow}$ and $s_{iz} = (1/2)(n_{i\uparrow} - n_{i\downarrow})$ being the charge and spin at the $i$–th site and $\tau = 0$. This type of characterization is useful and can be of help in understanding the electronic properties of a system. For instance, the SWF tells us the presence or absence of gaps or pseudogaps as $U$ increases, which is of fundamental importance in establishing the insulating or metallic character and possible transitions between them, say, the IHM. Likewise, the evolution of $c_k$ and $s_k$ with $U$, especially theirs peak at $k = \pi$, gives information about the charge or magnetic origin of the transitions.

A. The spectral-weight function.

As hinted before, it is just the structure of $A_k(\omega)$ at $k = \pi/2$ which accounts for the insulating or metallic character of the IHM. Hence, Fig 1 shows this quantity for three values of $U$ (recall that $t = 1$) so selected to exhibit the three fundamental regimes of the model. The calculation has been done for a chain of eighty sites with periodic boundary conditions at half filling and $\beta = 10$. Typically 150 time slices, two hundred warm sweeps and one thousand measurements were taken. At $U = 1$, a two-peak structure with a clear gap in between signals an insulating system. At $U = 2.25$, both peaks have overlapped developing a third peak just at the midpoint of the gap (which becomes the Fermi level). This three-peak structure clearly shows a metallic system. Finally, at $U = 4$ the central peak splits into two peaks leaving a gap in between. This four-peak structure signals again an insulating system which must be somehow of a different kind from the initial one (see below). As $U$ increases (not shown) the central gap widens and the four peaks go over into
FIG. 1: The spectral-weight function $A_k(\omega)$ for $k = \pi/2$ and $U/t$ ($t=1$) values lying in the three coupling regimes of the ionic Hubbard model. The QMC calculation has been made for a periodic chain of eighty sites at $\beta = 10$

a two-peak structure as $U \longrightarrow \infty$, the system becoming then a Mott insulator.

In order to estimate the approximate extension of the metallic region, Fig 2 shows the evolution of the spectral density at $k = \pi/2$ and $\omega = 0$ (the midgap) as $U$ increases. We see a maximum at $U_m = 2.25$ an onset threshold at $U_1 \simeq 1.75$ and a falloff with an approximate endpoint at $U_2 = 2.75$ eV leaving a zone of metallicity $U_2 - U_1 = 1$. Since this quantity may be size-dependent, we proceed to a finite-size scaling in order to approach the thermodynamic limit. Calculations made on chains of 8,12,16,80,120, and 160 sites show that $U_2 - U_1 = 1$ is roughly independent of size, but $U_m$ tends to go up, extrapolating to 2.50 when $1/N \longrightarrow 0$. Notice that only finite chains of $N = 4m$ sites should be used since only them have $k = \pi/2$ as an allowed wave vector. Chains of other lengths fail to detect the metallicity. In the thermodynamic limit, of course, all chains have a wave vector infinitesimally close to $\pi/2$

The three-peak structure responsible of the metallic phase disappears as soon as one
FIG. 2: $A_k(\omega)$ at $k = \pi/2$ (a=1) and E=0 (midgap which becomes the Fermi level) as U increases. Same calculations of Fig. 1

departs from $k = \pi/2$, showing a single mainly occupied peak at $k = (\pi/2) - \delta$ and a mainly empty peak at $k = (\pi/2) + \delta$ ($\delta = 2\pi/N$, $N$ being the number of sites). Hence the metallic peak should be visible in angle-resolved photoelectron spectroscopy and its inverse, but not in integrated measurements which give the DOS, Eq (8). Since the weight of that structure falls with $N$ (Fig 3), only a pseudogap with a sizeable DOS at the Fermi levels should be seen.

B. The charge and spin structure factors

Fig 4 finally displays the evolution of the peak of $c_k$ and $s_k$ at $k = \pi$ for increasing U. The charge factor consistently drops from a high value at $U = 1$, which signals a strong CDW in correspondence with a large ionicity (the fractional ionic character of the bond is
$FIC = 0.32$) which also falls down monotonically. The system, therefore starts as an ionic band insulator at small $U$. The spin structure factor starts close to zero, corresponding to a paramagnetic insulator, and monotonically increases with $U$, signaling an AF SDW of increasing amplitude. For large $U$, the system evolves into a Mott insulator with a strong AF SDW and a vanishingly small CDW, i.e., zero ionicity (neutral).

In the intermediate regime, $U_1 < U_2$, the system is both increasingly AF and neutral (decreasing ionicity, i.e., decreasing CDW). On the other hand, Table I displays a small sector of the density matrix ($n_{ij}^s = \langle c_{is}^+ c_{js} \rangle$), for $U = 2.25$ just the top and left $4 \times 4$ matrix, which is sufficient to show that the metallic state of this intermediate regime is dimerized. Thus $n_{12}^s > n_{23}^s$, etc, indicating that the sites (12), (34), and so on, form dimers. These dimers weaken for $U > U_2$ and tends to disappear as $U \to \infty$.

FIG. 3: Density of states for the same chain as Fig 1 for $U$ and number of sites $N=8,12,16$ and $80$. 
Our QMC study shows three coupling regimes in the ionic Hubbard model: (i) An ionic band insulator below $U = U_1$. (ii) An increasingly antiferromagnetic and dimerized metal which is gradually becoming neutral in the intermediate coupling regime $U_1 < U < U_2$. And (iii) an increasingly AF and neutral insulator whose dimerization, measured by $n_{12} - n_{23}$, is gradually dropping away for $U > U_2$. This last regime tends to a Mott insulator at $U \to \infty$.

A remark is here in order. Although the spectral-weight function at $k = \pi/2$ seems to hint a critical separation among the three coupling regimes (a threshold and an endpoint), the smooth behavior of all the integrated quantities (DOS, ionicity, energy, charge and spin structure factors, etc.) rather suggest a smooth interpolation between the three regimes which should be distinguished from true quantum phases with sharp, critical, separation among them.
To conclude, let us finally say that the results of our QMC calculations would be quite similar to those of Resta et al., Wilkens and Martin, etc, if the metallic zone reduced to a single point. On the other hand, they would also be quite close to those of Fabrizio et al. should the intermediate regime reported in this letter turn out to be insulating.

We acknowledge the financial support of the Spanish DGICYT through Project NPB 98-0683

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TABLE I. Upper-left $4 \times 4$ sector of the density matrix $n_{ij}^s = \langle c_{is}^+ c_{js} \rangle$

\begin{tabular}{cccc}
0.5477 & 0.2928 & 0.0109 & -0.0555 \\
0.2928 & 0.4523 & 0.2116 & -0.0133 \\
0.0109 & 0.2116 & 0.5477 & 0.2928 \\
0.0555 & -0.0133 & 0.2928 & 0.4523 \\
\end{tabular}