Quasiparticle spectral density of low-dimensional Hubbard Hamiltonians

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The spectral density of states of one- and two-dimensional Hubbard Hamiltonians is analyzed by means of Green's-function techniques. The procedure has been checked in the half-filled–band one-dimensional case by comparing it with the well-known solution of Lieb and Wu. When the ratio between the intrasite Coulomb interaction and the transfer integral is great enough, we find for subbands for both the one- and two-dimensional cases. Implications for Si(111) surfaces are commented on.

Correlation in narrow bands is a topic of current interest which has stimulated an increasing amount of attention to Hubbard Hamiltonians.[1] Lieb and Wu[2] have given an exact solution to the one-dimensional half-filled–band case. Other people have given alternative approaches[3-7]; these procedures yield good results for the ground-state energy and, in some cases, for the low-excited quasiparticles of the one-dimensional Hamiltonian,[8] and offer a way to solve Hubbard Hamiltonians of higher dimensions.[9]

The purpose of this Brief Report is to present new results for the spectral density of states of the one- and two-dimensional Hubbard Hamiltonians, extending other results[1-9] to the whole spectrum of electron excitations. In the two-dimensional case, we consider the Hubbard Hamiltonian recently introduced to analyze the correlation effects associated to the dangling-bond surface states of Si(111).[10-12]

The Hubbard Hamiltonian we are interested in reads as

$$\hat{H} = \sum_{i,\sigma} E_0 n_{i\sigma} + \sum_{i \neq j} t c_{i\sigma}^+ + \sum_i U n_{i\uparrow} n_{i\downarrow}$$

$$\equiv \hat{H}_0 + \sum_i U (n_{i\uparrow} n_{i\downarrow} - \langle n_{i\downarrow} \rangle n_{i\uparrow} - \langle n_{i\uparrow} \rangle n_{i\downarrow}) \ , \quad (1)$$

where t is the hopping interaction between nearest neighbors and U the intrasite Coulomb interaction. In Eq. (1), $\hat{H}_0$ represents the mean-field Hubbard Hamiltonian.

By using standard many-body techniques,[13] we can introduce the Green's function $G_{ij}(\omega)$ and the self-energy $\Sigma_{ij}(\omega)$, both quantities verifying the following equation:

$$[\omega \underline{I} - \underline{H}_0 - \underline{\Sigma}(\omega)] \underline{G}(\omega) = \underline{I} \ , \quad (2)$$

where $(\underline{H}_0)_{ij} = \langle i | \hat{H}_0 | j \rangle$, and $\underline{I}$ is the identity matrix.

In our procedure we look for an approximate self-energy $\underline{\Sigma}$. Our solution of $\underline{\Sigma}$ has been obtained with the following steps: (i) First, we neglect[12,14] any off-diagonal terms $\Sigma_{ij}^\sigma(\omega)$, $i \neq j$; (ii) Second, we determine $\Sigma_{ii}^\sigma(\omega)$ by following the argument given by Martín-Rodero et al.[15] This procedure yields

$$\Sigma_{ii}^\sigma(\omega) = \Sigma_{ii}^{\sigma(2)}(\omega) \Big/ 1 - \frac{(1 - \langle n_{i,-\sigma} \rangle) U + E_0 - \epsilon_{0,i}^\sigma}{\langle n_{i,-\sigma} \rangle (1 - \langle n_{i,-\sigma} \rangle) U^2} \Sigma_{ii}^{\sigma(2)}(\omega) \ ; \quad (3)$$

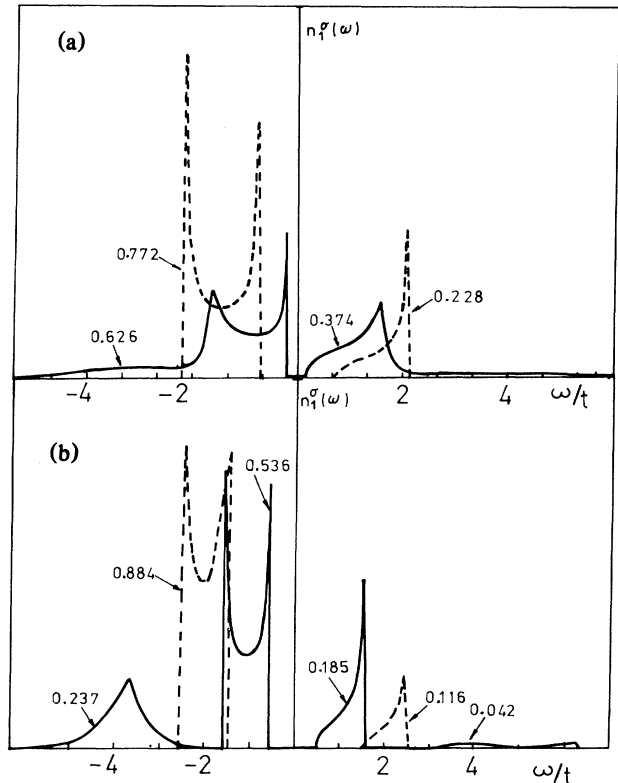here $\Sigma_{ii}^{\sigma(2)}(\omega)$ is the second-order term for the self-energy,

FIG. 1. Density of states for spin σ in atom 1, in the one-dimensional case, for (a) $U/t = 2.67$, (b) $U/t = 4$. Dashed line: HF solution. Figures give the strength of each band.

as calculated from Hamiltonian (1) by using the effective level $\epsilon_{0,i}$ instead of E_0. That level $\epsilon_{0,i}$ is adjusted to get self-consistency in the charges $\langle n_{i,\sigma} \rangle$, as calculated with the solution given by Eq. (2) and with the one obtained from the effective one-electron Hamiltonian[15]

$$\hat{H}_{\text{eff}} = \sum_{i,\sigma} \epsilon_{0,i}^{\sigma} n_{i,\sigma} + \sum_{\substack{i,j,\sigma \\ i \neq j}} t c_{i\sigma}^{+} c_{j\sigma} \ . \tag{4}$$

Once $\underline{\Sigma}(\omega)$ has been determined, Eq. (2) allows us to obtain the ground-state energy and the quasiparticle spectral density. We apply this method to one- and two-dimensional Hamiltonians. For the half-filled one-dimensional case, the ground state corresponds to an antiferromagnetic solution with two atoms, say, 1 and 2, in the unit cell. Then, by reasons of symmetry, we have the following relations:

$$\Sigma_{11}^{\uparrow}(\omega) = \Sigma_{22}^{\downarrow}(\omega) = -\Sigma_{11}^{\downarrow *}(-\omega) \ , \tag{5a}$$

$$n_1^{\uparrow}(\omega) = n_2^{\downarrow}(\omega) = n_1^{\downarrow}(-\omega) \ , \tag{5b}$$

and

$$\langle n_1^{\uparrow} \rangle = \langle n_2^{\downarrow} \rangle = 1 - \langle n_2^{\uparrow} \rangle = 1 - \langle n_2^{\downarrow} \rangle \ . \tag{5c}$$

A check to the method followed in this report is provided by comparing our results for the ground-state energy and the energy gap, with the exact ones given by Lieb and Wu

(LW).[2] In Table I, we present the values obtained in both cases for values of U/t corresponding to a region for which our procedure yields the lowest accuracy; the Hartree-Fock (HF) results are also given for comparison. Note that the results given by our method represent a substantial improvement over the HF solution, and give for both the ground-state energy and the energy gap an accuracy comparable with the one obtained with other approximate methods.[3,4] Moreover, it is worth commenting that for $U/t \simeq 2$ and 2.67, the asymptotic limits for the energy gap as obtained in LW[8] and HF methods practically apply:

$$\Delta(\text{LW}) = \frac{4}{\pi}(Ut)^{1/2} \exp\left[-\frac{2\pi t}{U}\right]; \quad \Delta(\text{HF}) = 8t \exp\left[-\frac{2\pi t}{U}\right];$$

in this region, our solution is quite close to the exact one, and this shows the good accuracy of our procedure. Although we have not been able to obtain in our method an analytic expression for the asymptotic behavior of Δ, our calculations show that the contributions coming from $\Sigma_{ii}^{\sigma}(\omega)$ and $\epsilon_{0,i}^{\sigma}$ are crucial to obtain that limit.

Once we have checked the accuracy of our method, we pass to consider the spectral density of quasiparticles for the same one-dimensional case. In Fig. 1 we give the total density of states for spin-up in atom 1, for $U/t = 2.67$ and 4, and compare it with a HF calculation. The most striking
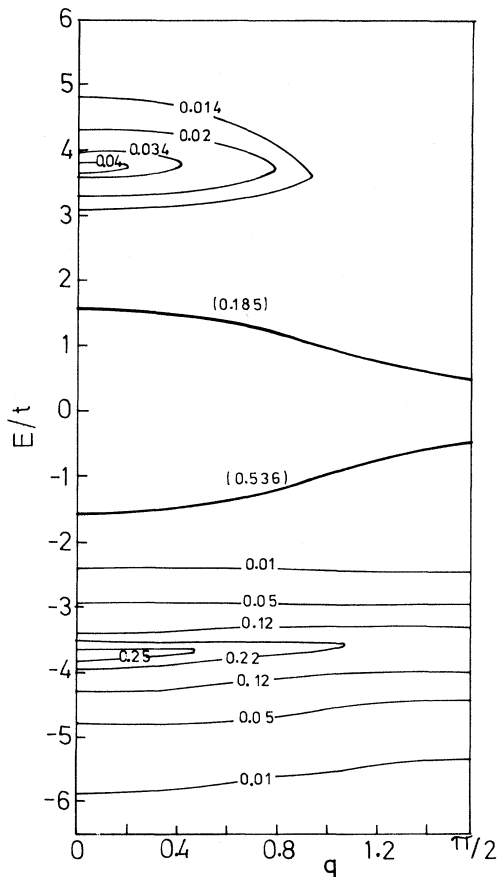

FIG. 2. Curves for constant values of the density of states, $n_1^{\uparrow}(q,E)$, in the one-dimensional case for $U/t = 4$. E is measured in units of t. In parenthesis we give the total density of states for each of the two sharp bands.
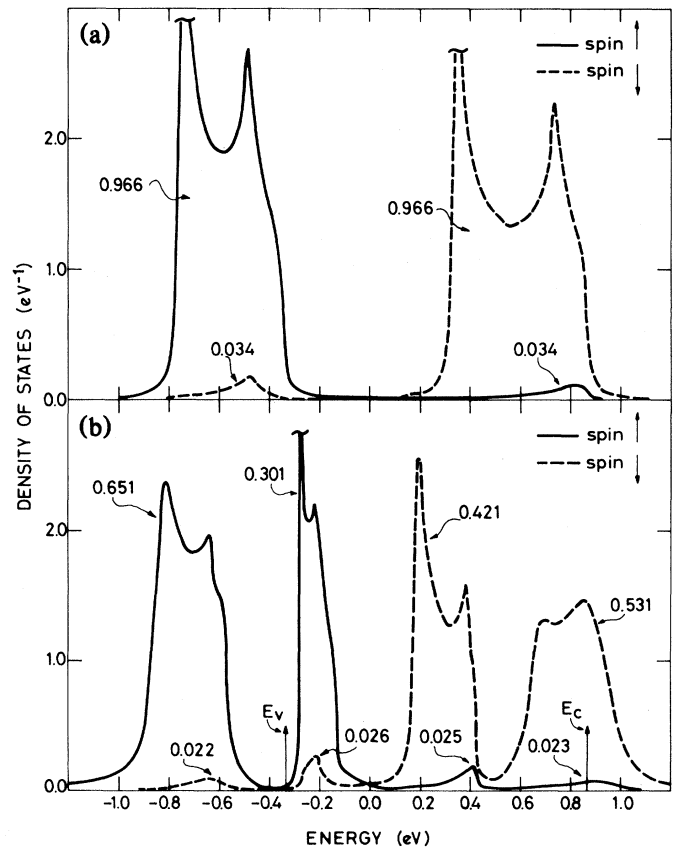

FIG. 3. Density of states in atom 1 for the two-dimensional case ($U = 1.17$ eV; $t = 0.15$ eV). $E_c \equiv$ conduction-band edge. $E_v \equiv$ valence-band edge. Figures give the strength of each band. Note that in this figure the different bands are not sharply defined because of the method of calculation. (a) HF solution, (b) our calculation.

TABLE I. Ground-state energy and energy gap (both in units of t) for different values of U/t. LW $\equiv$ Lieb and Wu (Ref. 2) solution. HF $\equiv$ Hartree-Fock solution.

U/t	Ground-state energy (E/t)			Energy gap (Δ/t)		
	LW	This work	HF	LW	This work	HF
2	−0.844	−0.826	−0.782	0.172	0.154	0.682
2.67	−0.737	−0.702	−0.651	0.451	0.358	1.455
4	−0.588	−0.500	−0.468	1.288	1.044	3.076

feature of our density of states is the appearance of four bands when we move from $U/t = 2.67$ to $U/t = 4$. This is due to a correlation effect which is lacking in the HF solution, where only two bands are found. Note that this effect only appears for U great enough, a limit for which two levels per spin are found at each atom; then, the four bands come from the two atoms in the unit cell. For this case, the HF solution gives an average of the two bands found in the valence or the conduction region.

In Fig. 2, the local density of states

$$n_1^{\uparrow}(q, \omega) = -\frac{1}{\pi} \mathrm{Im} G_{11}^{\uparrow}(q, \omega)$$

(q is the one-dimensional momentum) is shown for $U/t = 4$; this figure clearly illustrates the existence of four bands. It is of interest to point out that in the limit $U \rightarrow \infty$, we find that the strength of the two inner bands determining the energy gap goes to zero.

We now turn our attention to a two-dimensional case and consider the Hamiltonian recently proposed by some researchers[10-12] to analyze the correlation effects associated with the dangling bonds of the Si(111) surface. In this Brief Report we present the results obtained for the (2×1)-reconstructed surface as calculated by using the parameters given by Del Sole and Chadi[10]: $U = 1.15$ eV, $t = 0.10$ eV. In Fig. 3 we give the total density of states for the antifer-

romagnetic case as obtained by using our procedure as well as the HF solution, the case considered by Del Sole and Chadi.[10] Our results show that, for the given parameters, the system presents four bands in complete parallelism with the one-dimensional case. Note that the HF solution only gives two bands; in our solution, each of those bands is split into the two subbands of our valence and conduction region. It is of interest to remark that the more exact solution shows a much narrower gap than the HF case; this has also been found in the one-dimensional case (see Table I). Moreover, let us comment that for U great enough, the two inner bands determining the gap (with an increasingly small strength for $U/t \rightarrow \infty$) are the parallel, in the (2×1) anti-ferromagnetic case, of the Kondo-like peak appearing in the paramagnetic solution.[12,16] They can be interpreted as coming from the splitting of this Kondo-like peak, an effect due to the new symmetry of the (2×1) surface.

All these results show that the dangling bonds of the Si(111) surface represent a highly correlated electron gas,[9,10] and that for this system more accurate solutions than a HF one are needed if quantitative results, and even qualitative ones, are sought. The local spin-density functional[17] may give better results than the HF calculations, since correlation effects, as introduced in such a method, are likely to broaden the HF density of states, bringing the bandwidths into better agreement with our calculations.

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